Connecting via Winsock to STN

Q2-ALL, L1, L2, Z, Q, R1, R-ALL

Welcome to STN International! Enter x:x

LOGINID:SSPTANAG1626

PASSWORD:

NEWS HOURS

NEWS LOGIN

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
                 INSPEC enhanced with 1898-1968 archive
NEWS
         AUG 09
                 ADISCTI Reloaded and Enhanced
NEWS
         AUG 28
                 CA(SM)/CAplus(SM) Austrian patent law changes
         AUG 30
NEWS
         SEP 11
                 CA/CAplus enhanced with more pre-1907 records
NEWS
                 CA/CAplus fields enhanced with simultaneous left and right
NEWS
         SEP 21
                 truncation
                 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
      8
         SEP 25
NEWS
                 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
         SEP 25
NEWS
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10
         SEP 25
NEWS 11
         SEP 28
                 CEABA-VTB classification code fields reloaded with new
                 classification scheme
                 LOGOFF HOLD duration extended to 120 minutes
NEWS 12
         OCT 19
         OCT 19
                 E-mail format enhanced
NEWS 13
                 Option to turn off MARPAT highlighting enhancements available
         OCT 23
NEWS 14
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 15
         OCT 23
                 multiple databases
                 The Derwent World Patents Index suite of databases on STN
NEWS 16
         OCT 23
                 has been enhanced and reloaded
                 CHEMLIST enhanced with new search and display field
NEWS 17
         OCT 30
                 JAPIO enhanced with IPC 8 features and functionality
         NOV 03
NEWS 18
NEWS 19
         NOV 10
                 CA/CAplus F-Term thesaurus enhanced
                 STN Express with Discover! free maintenance release Version
NEWS 20
        NOV 10
                 8.01c now available
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 21
         NOV 20
                 additional databases
NEWS 22
         NOV 20
                 CA/CAplus to MARPAT accession number crossover limit increased
                 to 50,000
         DEC 01
                 CAS REGISTRY updated with new ambiguity codes
NEWS 23
                 CAS REGISTRY chemical nomenclature enhanced
NEWS 24
         DEC 11
                 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25
         DEC 14
                 GBFULL and FRFULL enhanced with IPC 8 features and
NEWS 26
         DEC 14
                 functionality
                 CA/CAplus pre-1967 chemical substance index entries enhanced
         DEC 18
NEWS 27
                 with preparation role
NEWS 28
         DEC 18
                 CA/CAplus patent kind codes updated
                 MARPAT to CA/CAplus accession number crossover limit increased
NEWS 29
         DEC 18
                 to 50,000
                 MEDLINE updated in preparation for 2007 reload
NEWS 30
         DEC 18
              NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
NEWS EXPRESS
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
```

STN Operating Hours Plus Help Desk Availability

Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8 NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 14:02:27 ON 21 DEC 2006

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:03:05 ON 21 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0 DICTIONARY FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10510026RTRexpand.str

```
chain nodes :
7  9  18  19  22  23
ring nodes :
1  2  3  4  5  10  11  12  13  14  15
chain bonds :
1-22  1-23  2-7  4-18  4-19  5-9  9-10
ring bonds :
1-2  1-5  2-3  3-4  4-5  10-11  10-15  11-12  12-13  13-14  14-15
exact/norm bonds :
1-2  1-5  1-22  1-23  2-3  2-7  3-4  4-5  4-18  4-19  5-9
exact bonds :
9-10
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15
```

G1:H,CH3

G2:0,S

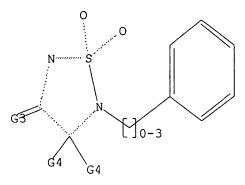
G3:0,S,N

G4:H,CH3

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0, S

G3 O, S, N

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 14:03:30 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 68 TO ITERATE

50 ANSWERS 100.0% PROCESSED 68 ITERATIONS

SEARCH TIME: 00.00.01

ONLINE **COMPLETE** FULL FILE PROJECTIONS:

COMPLETE BATCH

1854 866 TO PROJECTED ITERATIONS: 576 TO 1424 PROJECTED ANSWERS:

50 SEA SSS SAM L1 L2

=> s l1 full

FULL SEARCH INITIATED 14:03:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -1124 TO ITERATE

766 ANSWERS 1124 ITERATIONS 100.0% PROCESSED

SEARCH TIME: 00.00.01

766 SEA SSS FUL L1 1.3

=> fil hcaplus

TOTAL SINCE FILE COST IN U.S. DOLLARS SESSION

ENTRY

166.94 167.15 FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 14:03:44 ON 21 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Dec 2006 VOL 145 ISS 26 FILE LAST UPDATED: 20 Dec 2006 (20061220/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 33 L3

=> d ed ibib abs hitstr 1-33

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 03 Aug 2006 ACCESSION NUMBER: 2006:765251 HCAPLUS DOCUMENT NUMBER: 145:211037

145:211037
Preparation of pyrarolyl aryl ureas as modulators of the protein kinase activation state for treatment of inflammation and hyperproliferative diseases flynn, Daniel L., Petillo, Peter A. Deciphera Pharmaceuticals, LLC, USA PCT Int. Appl., 305pp.
CODEN: PIXXD2 TITLE:

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.					KIND DATE				APPLICATION NO.						DATE			
						-									-			
wo	2006	0810	34		A2		2006	0803		WO 2	005-	US 47	597		2	0051	223	
wo	2006	0810	34		A3		2006	1123										
	w:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FĮ,	GB,	GD,	
		GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	J₽,	KE,	KG,	KM,	KN,	KP,	ΚŔ,	
		ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MĢ,	MK,	MN,	MW,	ΜX,	
		MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RΟ,	RU,	SC,	SD,	SE,	
		SG,	SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	ΤZ,	UΑ,	UG,	US,	UZ,	vc,	
					ZM,													
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
		CF,	ÇG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	B₩,	GH,	
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	52,	ΤZ,	υG,	ZM,	ZW,	AM,	ΑZ,	BY,	
		KG.	KZ.	MD,	RU,	TJ.	TM											

NG, KZ, MD, RU, TJ, TM PRIORITY APPLN. INFO.: US 2004-638987P P 20041223

OTHER SOURCE(S):

MARPAT 145:211037

Novel compds. and methods of using those compds. for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and diseases
characterized by hypervascularization are provided. In a preferred

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

 $\begin{array}{lll} 872171-37-4 & HCAPLUS \\ Urea, & N-\left[3-\left(1,1-\dim (+hy)\right)-1-\left[3-\left[\left(3R\right)-3-methy\right]-1,1-\dim (+hy)-4-oxo-1,2,5-c-hidaiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) & (CA INDEX NAME) \\ \end{array}$

Absolute stereochemistry.

872171-57-8 HCAPLUS

overly-2-ro mering 2-Naphthalenecarboxanide, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiozolidin-2-yl)methyl]phenyl]-1H-pyrazo1-5-yl]- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) embodiment, the compds. of the invention modulate the activation state of p38 kinase protein, abl kinase protein, bcr-abl kinase protein, braf kinase protein, bcr pr

45 nM. 872171-35-2P, 1-(5-tert-Butyl-2-(3-((5)-3-methyl-1,1,4-trioxo-ΙT

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-{[(R)-3-nethyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl}-3-(naphthalen-1-yl)urea 872171-63-6P, 1-{5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl}-3-(4-chlorophenyl)urea 872171-73-8P, 1-{5-tert-Butyl-2-{3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-methoxynaphthalen-1-yl)urea RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(p38 kinase inhibitor; preparation of pyrazolyl aryl ureas as

(p38 Kinase inniaros. perparation of the protein kinase activation state for treatment of inflammation and hyperproliferative diseases)

RN 872171-35-2 MCAPLUS

CN Urea. N-[3-(1.1-dimethylethyl)-1-[3-{(35)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyllphenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9C1) (CA INDEX NAME)

872171-63-6 HCAPLUS
Urea, N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

872171-73-8 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl|phenyl|-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-39-6 HCAPLUS Urea, N- $\{3-\{1,1-\text{dimethylethyl}\}-1-\{3-\{\{5-\{(4-\text{methoxyphenyl}\}\text{methyl}\}-1,1-\{3-\{(5-\{(4-\text{methoxyphenyl}\}\text{methyl}\}-1,1-\{(4-\text{methoxyphenyl}\}\text{methyl}\}-1,1-\{(4-\text{methoxyphenyl}\}\text{methyl}\}-1,1-\{(4-\text{methoxyphenyl}\}\text{methyl}\}-1,1-\{(4-\text{methoxyphenyl})\}\text{methyl}\}-1,1-\{(4-\text{methoxyphenyl})\}$

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl}-1H-pyrazol-5-yl}-N'-{4-fluorophenyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-[5-tert-Butyl-2-[3-[[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-(4],1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-[4-fluorophenyl)urea RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of pyrazolyl aryl ureas as modulators of protein kinaso activation state for treatment of inflammation and hyperproliferative diseases)
RN 872171-36-3 HCAPLUS
CN Urea, N-[3-[1,]-dimethylethyl)-1-[3-[(3R)-5-[4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

L4 ANSMER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 28 Jul 2006
ACCESSION NUMBER: 2006:739358 HCAPLUS
DOCUMENT NUMBER: 145:377543
TITLE: 15othiazolidinone heterocycles as inhibitors of protein tyrosine phosphatases: Synthesis and structure-activity relationships of a peptide

SCRUCLURE-ACTIVITY relationships of a peptide
Yue, Eddy W.: Nayland, Brian: Douty, Brent: Crawley,
Mathaw L.; McLauphlin, Erin: Takvorian, Amy;
Wasserman, Zelda: Bower, Michael J.: Wei, Min: Li,
Yanlong: Ala, Paul J.: Gonneville, Lucie: Wynn,
Richard: Burn, Timothy C.; Liu, Phillip C. C.: Combs,
Andrew P.
Discovery Chemistry, Experimental Station, Incyte
Corporation, Wilmington, DE, 19880, USA
Bioorganic & Medicinal Chemistry (2006), 14(17),
5833-5849
CODEN: BMECEP; ISSN: 0968-0896
Elsevier B.V.
Journal
English

CORPORATE SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: GI

Oxo- and trioxo-substituted isothiazolidinylphenylalanines are prepared

tyrosine mimetics by Suzuki coupling reactions of

chloroisothisolidinones
 and chlorodioxoisothisolidinones with N-Boc-4-borono-L-phenylalanine
 and chlorodioxoisothisolidinones with N-Boc-4-borono-L-phenylalanine
 derivs. The isothiazolidinylphenylalanines (with or without subsequent
 hydrogenation) are incorporated into dipeptides prepared as human protein
 tyrosine phosphatase 18 (PFPIB) inhibitors such as I. Of the compds.
 tested, I is the most potent inhibitor of PTPIB with an IC50 value of 40
 nM; the corresponding mixture of isothiazolidinone diastereomers inhibits
 PTPIB with an IC50 value of 80 nM, and the separated
 (R)-isothiazolidinone
 diastereomer inhibits PTBIB with an IC50 value of 15 5 nM; the related

usothiazolidinone diastrecomer inhibits PTBlB with an IC50 value of 15.5 µM; the related dispercioner inhibits PTBlB less potently than either I or the

mixture of isothiazolidine diastereomers containing I. Crystal structures of a

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-21-8 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(SCI) (CA INDEX NAME)

 $850315-23-0 \quad HCAPLUS \\ L-Phenylalaninamide, \quad N-\left\{\{4-methoxyphenyl\}acetyl\}-L-phenylalanyl-4-\left\{1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl\}-N-pentyl- (9CI) . (CA INDEX NAME)$

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) dioxothiazolidinone-substituted dipeptide and a dioxoisothiazolinone-substituted dipeptide bound to PTPIB are detd. by X-ray crystallog,: the low energy conformation found by ab initio calcus, for the satd. heterocycle more closely approaches the conformation obtained upon

heterocycle more closely approaches the Contribution Solution of Schmiding
to PTPIB than that of the unsaid. heterocycle.

18 550315-22-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of isothiazolone- and dioxoisothiazolone-substituted phenylelanine-containing dipeptide amides and their activities as

"PTP1B inhibitors)
850315-22-9 HCAPLUS
L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl}-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-20-7P 850315-21-8P 850315-23-0P
910606-95-0P 910606-97-2P
Rt: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of isothiazolone- and dioxolothiazolone-substituted
phenylalanine-containing dipeptide amides and their activities as

n
PTP1B inhibitors)
850315-20-7 HCAPLUS
Carbamic acid, ([15]-1-[[4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thladiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

910606-95-0 HCAPLUS Benzenepropanamide, α -amino-4-[1,1-dioxido-4-oxo-5-{phenylmethyl}-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (αS) -, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 910606-94-9 CMF C23 H30 N4 O4 S

Absolute stereochemistry

CRN 76-05-1 CMF C2 H F3 O2

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 910606-97-2 HCAPLUS

910606-97-2 HCAPLUS
L-Phenylalaninamide,
senylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]-N-pentyl-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CRN 910606-96-1 CMF C32 H39 N5 O5 S

Absolute stereochemistry.

СМ

REFERENCE COUNT:

THERE ARE 39 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

(Continued) ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Title compds. (RIXj)mA(NH)pLn(NH)pDEqYtO [I: wherein Rl = (un)substituted (hetero)aryl: X, Y = independently O, S, NR6, NR6SO2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene,

O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h

1-4; $A = \{un\}$ substituted aryl, hetero(bi)cyclyl; $D = \{un\}$ substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; $E = \{un\}$ substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2;

m, n, p, q, t = independently 0, 1; Q = $\{un\}$ substituted heterocycly1, Ph, etc.: R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions]

prepared as p38 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p38 kinase protein comprises the step of contacting the α -C helix, the α -D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation

claimed, prepns. and/or characterization data for .apprx.150 examples of

and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester using 10% Pd/C in EtOH provided

propionate, which was treated with NaNO2 in the presence of 6N HCl and ShCl2e2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-(3-(3-ctr-butyl-5-amino-1H-pyrazole-1-yl)phenyl)propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction

LiOH in THF/MeOH/H2O provided the urea II. In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase

IC50 of 45 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data). 872171-35-2P, 1-[5-tert-Butyl-2-{3-{[(S)-3-methyl-1,1,4-trioxo-ΙT

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-cert-Butyl-2-[3-[(R)-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrezol-3-y1]-3-(naphthalen-1-y1)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 29 Dec 2005
ACCESSION NUMBER: 2005:1346235 HCAPLUS
DOCUMENT NUMBER: 144:88279
TITLE: Preparation of 1-pyrazolyl-3-phenylurea p38 MAP
kinase

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

inhibitors as antiinflammatory medicaments
Flynn, Daniel L.; Petillo, Peter A.
USA
USA
U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S.
Ser. No. 746,460.
CODEN: USXXCO
Patent

LANGUAGE:	English						
FAMILY ACC. NUM. COUNT:	4						
PATENT INFORMATION:							
PATENT NO.	KIND DATE	APPLICATION NO.					
US 2005288286	A1 20051229	US 2004-886329	20040706				
US 2004180906	A1 20040916	US 2003-746460	20031224				
	B2 20061205						
		WO 2005-US23100	20050630				
WO 2006014290							
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BW,	BY, BZ, CA, CH,				
CN, CO, CR,	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,				
GE, GH, GM,	HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KM, KP, KR, KZ,				
LC, LK, LR,	LS, LT, LU, LV,	MA, MD, MG, MK, MN,	MW, MX, MZ, NA,				
NG, NI, NO,	NZ, OM, PG, PH,	PL, PT, RO, RU, SC,	SD, SE, SG, SK,				
SL, SM, SY,	TJ, TM, TN, TR,	TT, TZ, UA, UG, US,	UZ, VC, VN, YU,				
ZA, ZM, ZW							
RW: AT, BE, BG,	CH, CY, CZ, DE,	DK, EE, ES, FI, FR,	GB, GR, HU, IE,				
IS, IT, LT,	LU, MC, NL, PL,	PT, RO, SE, SI, SK,	TR, BF, BJ, CF,				
CG, CI, CM,	GA, GN, GQ, GW,	ML, MR, NE, SN, TD,	TG, BW, GH, GM,				
KE, LS, MW,	MZ, NA, SD, SL,	SZ, TZ, UG, ZM, ZW,	AM, AZ, BY, KG,				
KZ, MD, RU,	TJ, TM						
PRIORITY APPLN. INFO.:		US 2003-746460	A2 20031224				
		US 2002-437304P	P 20021231				
		US 2002-437403P	P 20021231				
		US 2002-437415P	P 20021231				
		US 2002-437487P	P 20021231				
		US 2003-463804P	P 20030418				
		US 2004-886329	A 20040706				

OTHER SOURCE(S):

MARPAT 144:88279

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl}-3-{4-methoxynaphthalen-1-yl}urea RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

Absolute stereochemistry.

872171-37-4 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-{3-{{(3R}-3-methyl-1,1-dioxido-4-oxo-1,2,5-chiadiazoltdin-2-yl]methyl]phenyl}-1H-pyrazol-5-yl}-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry

872171-57-8 HCAPLUS

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-Naphthalanecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9CI) (CA INDEX NAME)

872171-63-6 HCAPLUS Urea, N-(4-chlorophonyl)-N'-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phonyl]-lH-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-[5-tert-Butyl-2-(3-[[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3yl]-3-(naphthalen-1-yl]wrea 872]11-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenryl]-1,1,4-trioxo-[1,2,5]thiadiazolidin-2yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-[4-fluorophenyl]wrea
872]11-49-8P, 1-[5-tert-Butyl-2-[3--[[1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4fluorophenyl]wrea
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation of (pyrazolyl) (phenyl)wrea p38 kinase inhibitors as antinflammatory agents)
872[1]-36-3 HCAPLUS
CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-[{(3R)-5-[(4-methoxyphenyl)methyl]-3methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1Hpyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-39-6 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[[5-((4-methoxyphenyl)methyl)-1,1-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]]methyl]phenyl]-lH-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-fluorophenyl)- (9C1) (CA INDEX NAME)

872171-49-8 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 2-A

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Aug 2005
ACCESSION NUMBER: 2005:904352 HCAPLUS
DOCUMENT NUMBER: 143:248386
TITLE: Preparation of substituted axole derivatives for treating diseases mediated by PTPase activity
INVENTOR(S): Mjalli, Addran M. M.: Polisetti, Dharma R.: Subramanian, Govindan; Quada, James C.: Atimilli, Murty N.: Yarragunta, Ravindra R.; Andrews, Robert Xie, Rongyuan
USA
U.S. Pat. Appl. Publ., 204 pp.
CODEN: USXXCO
Patent
English 1 PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

OTHER SOURCE(S):

MARPAT 143:248386

W 20050211

WO 2005-US4590

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

The title compds. I [a, b = 0-2; W = 0, S, NR2 (wherein R2 = alkyl,

); $R_1 = H$, halo, CN, etc.; L1 = a direct bond, (un)substituted NHCO, NHSO2, etc.; Ar1 = (un)substituted (hetero)aryl, fused cycloalkylaryl, etc.; Ar2 = (un)substituted (hetero)arylene, fused arylcycloalkylene, etc.; L2 = CH2, O, alkylene, etc.; which can be useful as inhibitors of protein tyrosine phosphatases and thus can be useful for the management, treatment, control, or the adjunct treatment of diseases mediated by PTPase activity such as type I diabetes and type II diabetes, were

prepared Thus, treating

Thus, treating
4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1Himidarole with Me bromoacetate followed by ester hydrolysis afforded 56t
(4-{2,4-dichlorophenyl}-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1H-imidarol-1yl)acetic acid. The representative compds. I were tested for inhibition
of PTP-1B. In general, the exemplified compds. I may inhibit PTP-1B with
ICSO of less than 20 µM. The pharmaceutical compns. comprising the
compds. I, and their use in treating human or animal disorders are also
disclosed.

IT 861243-91-8D 863245-51-2D 863245-74-3D

qisclosed. 863243-91-8P 863245-57-2P 863245-74-3P 863246-05-3P

863246-05-JP RI: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TMU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) [preparation of substituted azole derivs. for treating diseases

(preparation of Substitutes 1.1)

PTPase activity)

RN 65243-91-8 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-{2,4-dichlorophenyl}]-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4,4-dimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-57-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-{2,4-dichlorophenyl}]-2-[(1E)-2-{3'-trifluoromethoxy}](1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

863245-74-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-([4-(2,4-dichlorophenyl)-2-[(1E)-2-(2-1)-2-(1-1)

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9C1) (CA INDEX NAME)

Double bond geometry as shown.

 $863246-05-3 \quad HCAPLUS \\ Benzoic acid, \quad 4-\{[4-(2,4-dichloropheny]]-2-\{[1E]-2-[4-(1,1-dioxido-4-oxo-1,2,5-chiadiezolidin-2-y]] \\ phenyl]-1H-imidazol-1-y] \\ methyl ester (9CI) (CA INDEX NAME)$

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

C1

861243-80-5P 863243-92-9P 863243-91-0P
863243-94-1P 863243-95-2P 863243-95-7P
863224-06-0P 863244-07-9P 863243-0P
8632244-13-7P 863244-47-7P 863243-91-0P
863224-52-4P 863244-53-5P 863245-52-4P
863224-52-0P 863245-58-3P 863245-52-4P
8632245-50-1P 863245-61-8P 863245-52-9P
8632245-61-0P 863245-61-8P 863245-63-9P
8632245-61-0P 863245-64-1P 863245-63-P
8632245-70-9P 863245-71-0P 8632245-67-P
8632245-71-0P 863245-71-0P 863245-71-0P
8632245-71-0P 863245-71-0P 863245-71-0P
8632245-71-0P 863245-71-0P 863245-71-0P
8632245-02-3P 863246-03-3P 863246-03-1P
8632245-03-3P 863246-11-1P 863246-10-7P
8632245-03-3P 863246-11-1P 863246-10-7P
8632245-03-3P 863246-11-1P 863246-10-7P
8632246-10-0P 863246-11-1P 863246-10-7P
8632287-03-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Uses)

(Uses)

(preparation of substituted azole derivs. for treating diseases mediated by PTPase activity)
RN 863243-80-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-difluorophenyl)-2-[(1E)-2-(3'-(trifluoromethyl)[1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

PAGE 2-A

PAGE 1-A

863243-94-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2-chlorophenyl)-2-[(1E)-2-[3'-ttrifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-92-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-H-inidazol-1-yl]methyl]phenyl]-2,4,4-trimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863243-93-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-phenyl-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide [9C1] (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-95-2 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-{4-[{4-(4-chloropheny1)-2-{(1E}-2-{3'-trifluoromethyl)[1,1'-bipheny1}-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-05-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-06-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[(4-(3,4-dichlorophenyl)-2-[(1E)-2-{3'-(trifluoromethyl)[1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-07-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl}-1H-inidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 (methylsulfonyl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazol-1-yl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-47-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[[3-(trifluorophenyl)]phenyl]methyl]-lH-imidazol-1-yl]methyl!phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 663244-51-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-{[4-(2,4-dichlorophanyl)-2-[2-[4-(trifluoromethyl)phenyl]-thyl]-1H-imidazol-1-yl]methyl]phenyl}-,

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Double bond geometry as shown.

RN 863244-08-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2-chloro-4-fluorophenyl)-2-[[1E]-2[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-13-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[[3'-

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-S2-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
C14-[[4-[2,4-dichiorophenyl]-2-[2-[2-fluoro-4(trifluoromethyl)phenyl]-i,1-dioxide (9CI) (CA INDEX MAME)
1,1-dioxide (9CI) (CA INDEX MAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 863244-53-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-[2,4-dichloropheny1]-2-[2-[3'-trifluoromethoxy][1,1'-bipheny1]-4-y1]ethy1]-1H-imidazol-1-y1]methy1]pheny1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-56-1 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiarolidin-3-one, 5-{4-{[2-{(1E)-2-{3'-chloro[1,1'-biphenyl]-4-yl)ethenyl}-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl)methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-60-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(1-

methylethoxy) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-61-8 HCAPLUS 1,2,5-Thladiazolidin-3-one, 5-[4-[{4-{2,4-dichlorophenyl}}-2-[(1E)-2-[4'-[(1-methylethyl)thio][[,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-[4-[[2-[(1E)-2-[3].5]bis[trifluoromethy]][1,1]-bipheny]]-4-y]etheny]]-4-(2,4-dichloropheny]]1H-imidazol-1-yl]methyl]pheny]]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-58-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{4-{[4-(2,4-dichlorophenyl)-2-{(1E)-2-(2'-fluoro-5'-propoxy[1,1'-biphenyl]-4-yl]ethenyl}-1H-inidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-59-4 HCAPLUS

ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl]methyl]phenyl]-, l,l-dioxide (9CI) (CA INDEX NAME)

uble bond geometry as shown.

863245-62-9 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 5-{4-[[4-(2,4-dichlorophenyl)-2-{(1E)-2-{4'-(1,1-dimethylethyl)[1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:continuous} \begin{array}{lll} 863245-63-0 & HCAPLUS \\ 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dimehy]ethyl]-5'-methyl[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) \\ \end{array}$

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-64-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{4-[(2-[(1E)-2-[4-(5-chloro-2-thienyl)phenyl)-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-66-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{2-[(1E)-2-[4-(5-acetyl-2-thienyl)phenyl)-thenyl]-4-(2,4-dichlorophenyl)-lH-imidazol-1-yl]methyl]phenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-69-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-(2,4-dichlorophenyl)-2-{(1E)-2-[3'-(4,4,4-trifilorobutoxy)(1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-70-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-(2,4-dichlorophenyl)-2-[{1E}-2-[3'-

fluoro-4'-(4,4,4-trifluorobutoxy){1,1'-biphenyl}-4-yl]ethenyl}-1H-imiderol-l-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

663245-67-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2'-fluoro-5'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-68-5 HCAPLUS 1,2,5-Thiadtazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl]-2-[(1E)-2-[3'-4],3-dinethylbutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-71-0 HCAPLUS
Carbamic acid, [4'-[[1E]-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl]-4-fluoro[1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:continuous} $863245-72-1$$ KCAPLUS $1,2,5-$\text{Thiadaeolidin-3-one, } 5-[4-[\{4-(2,4-\text{dichloropheny}1\}-2-\{(1E)-2-\{3'-(\text{trifluoromethy}1\}-1,1'-\text{bipheny}1\}-4-y1]\text{etheny}1]-1H-imidaeol-1-y1]methy1]pheny1]-4-methy1-, 1,1-dioxide (9CI) (CA INDEX NAME)$

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-75-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-{2,4-dichlorophenyl}-2-[{1E}-2-{2-1}]}

fluoro-4-(trifluoromethyl)phenyl)ethenyl]-1H-imidazol-1-yl]methyl)phenyl]-2-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-78-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[[1E]-2-[4-(4,4,4-trifluorobutoxy)phenyl]-thenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide [9CI] (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(trifluoromethyl)phenoxy)phenyl]ethenyl]-1H-imidazol-1-yl}methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-03-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{{4-(2,4-dichlorophenyl)-2-{(1E)-2-{3'-(methylsulfonyl){1,1'-biphenyl}-4-yl}ethenyl)-1H-imidazol-1-yl}methyl}phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-04-2 HCAPLUS

GOJZWO-WW-E HOAFLUS 1,2,5-Thiediazolidin-3-one, 5-[4-[(1E)-2-[4-(2,4-dichlorophenyl)-1-ethyl-1H-imidazol-2-yl]ethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Double bond geometry as shown.

RN 863245-80-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[4-[4-

{1,1-dimethylethyl)phenoxy]phenyl]ethenyl]-lH-imidazol-l-yl]methyl]phenyl], l,1-dioxide (9CI) {CA INDEX NAME}

Double bond geometry as shown.

RN 863245-82-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-[4-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-06-4 HCAPLUS Benzoic acid, 4-[[4-{2,4-dichlorophenyl}]-2-[(1E)-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]ethenyl]-1H-imidazol-1-yl]methyl}- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-07-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[4-{2,4-dichlorophenyl}-2-[{1E})-2-[3'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-09-7 RCAPLUS
Carbamic acid, (4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)-1H-imidazol-2-yl)ethenyl][(1,1'-biphenyl)-3-yl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-10-0 HCAPLUS Carbamic acid, [4'-[4]:]-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]methyl]-lh-imidazol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Double bond geometry as shown.

863246-13-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-phenoxyphenyl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide

(CA INDEX NAME)

Double bond geometry as shown.

863246-15-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[[1E]-2-[3'-

(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-2-methylphenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 863246-11-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1-

methylethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863246-12-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichlorophenyl)-2-[(1E)-2-(3'-methyl[1,1'-biphenyl]-4-yl)ethenyl]-H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-16-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl)],1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-4-propyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863287-03-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,6-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl[methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 863247-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Reactant or reactant or rea

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-89-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

692764-94-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA NNDEX NAME)

852835-44-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER S OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 May 2005
ACCESSION NUMBER: 2005:378875 HCAPLUS
100CUMENT NUMBER: 143:19267
Structure-based design of protein tyrosine phosphatasp-18 inhibitors
Black, Emma: Breed, Jason; Breeze, Alexander L.; Embrey, Kevin; Garcia, Robert; Gero, Thomas W.; Godfrey, Linda; Kenny, Peter W.; Morley, Andrew D.; Minshull, Claire A.; Pannifer, Andrew D.; Read, Jon; Rees, Amanda; Russell, Daniel J.; Toader, Dorin; Tucker, Julie
AstraZeneca, Cheshire, SK10 4TG, UK
Bioorganic 4 Medicinal Chemistry Letters (2005), 15(10, 2501-2507 CODEM: BMCLEB; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE(S):

MENT TYPE: Journal
UAGE: English
R SOURCE(S): CASREACT 143:19267
Using structure-based design, a new class of inhibitors of protein
tyrosine phosphatase-18 (PTPE) has been identified, which incorporate

1,2,5-thiadiazolidin-3-one-1,1-dioxide template.
692765-80-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) or reagent)
(structure-based design of protein tyrosine phosphatase-1B inhibitors)
692765-80-3 KCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA
INDEX NAME)

IT

612530-44-6P 692764-89-9P 692764-94-6P 852835-44-0P 852835-45-1P RL: PRC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (structure-based design of protein tyrosine phosphatase-1B inhibitors) 612530-44-6 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852835-45-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 22 Apr 2005 ACCESSION NUMBER: 2005:347030 HCAPLUS DOCUMENT NUMBER: 142:4(11350 TITLE: Practice)

142:4(1350
Preparation of 1-oxo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins Combs, Andrew P.: Yue, Eddy Wai Tsun; Bower, Michael Jason; Zhu, Wenyur Crawley, Mathew Lantz; Sparks, Richard Bruce; Pruitt, James Russell; Takvorian, Amy Incyte Corporation, USA
PCT Int. Appl., 529 pp.
CODEN: PIXXD2
Patent
English
1 INVENTOR(S)

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	NO.				ICATION !	10.	DATE				
	035551				004-US33	212	20041007				
WO 2005	035551	A3	20060908								
W:	AE, AG, AL,	AM, AT	, AU, AZ,	BA, BB,	BG, BR,	BW, BY	, BZ, CA, CH,				
	CN. CO. CR.	CU, CZ	, DE, DK,	DM, DZ,	EC, EE,	EG, ES	, FI, GB, GD,				
	GE, GH, GM,	HR, HU	, ID, IL,	IN, IS,	JP, KE,	KG, KP	, KR, KZ, LC,				
	LK, LR, LS,	LT, LU	, LV, MA,	MD, MG,	MK, MN,	MW, MX	, M2, NA, NI,				
	NO, NZ, OM,	PG, PH	, PL, PT,	RO, RU,	SC, SD,	SE, SG	, SK, SL, SY,				
	TJ, TM, TN,	TR, TT	, TZ, UA,	UG, US,	UZ, VC,	VN, YU	, ZA, ZM, ZW				
RW:	BW, GH, GM,	KE, LS	, MW, M2,	NA, SD,	SL, SZ,	TZ, UG	, ZM, ZW, AM,				
	AZ, BY, KG,	KZ, MD	, RU, TJ,	TM, AT,	BE, BG,	CH, CY	, CZ, DE, DK,				
	EE. ES. FI.	FR, GB	, GR, HU,	IE, IT,	LU, MC,	NL, PL	, PT, RO, SE,				
	SI. SK. TR.	BF, BJ	, CF, CG,	CI, CM,	GA, GN,	GQ, GW	, ML, MR, NE,				
	SN, TD, TG										
US 2005	272778	A1	20051208	US 2	004-9603	4 4	20041007				
US 7141	596	B2	20061128								
PRIORITY APP	LN. INFO.:			US 2	003-5100	02 P	P 20031008				
				US 2	003-5293	72 P	P 20031211				
				110 3	004-6005	069	P 20040811				

OTHER SOURCE(S):

CASREACT 142:411350; MARPAT 142:411350

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention provides 1-oxo and 1,1-dioxoisothiazolones (shown

I-IV: also isothiazolidinone analogs of I-IV with R16 and R17 in place of R15 and R2 as a substituent at the 5 position of the isothiazolidinone ring; variables defined below; e.g. V) and related compds. that can modulate (no data) the activity of a target protein, such as a phosphatase, that selectively binds phosphorylated peptides or proteins. The present compds. can be useful (no data) in treating diseases or

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]biphenyl-4-sulfonamide 850315-36-5P 850315-40-1P, 4-Brono-N-[(18)-2-(4-(1)-1d-idoxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-48-5P, N-[(18)-2-(4-(1,1-bioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-3,5-bis[trifluoromethyl)benzenesulfonamide trifluoroacetate 850315-48-9P, N-[(18)-2-[4-(1,1-bioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-63-8P, N-[(18)-2-[3-chioro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-bundin-2-yl)phenyl-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)biphenyl-4-sulfonamide trifluoroacetate 850315-65-0P 850315-69-4P

, mo+N-{{15}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2omo-N-[(15)-2-[3-chloro-4-(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-73-0P ,N-[(15)-2-[3-chloro-4-(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis[trifluoromethyl]benzenesulfonamide trifluoroacetate 850327-65-0P 850327-67-2P, N-[(15)-1-(5-Chloro-1H-

benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl}-2-cyanobenzenesulfonamide trifluoroacetate 850327-69-4P, N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-71-8P,

N-{(1S)-1-(5-Chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-73-0P, N-{(1S)-1-(5-Chloro-1H-

critiuoroacetate esuszi-i-s-uv, N-([15]-1-[5-thiofo-in-benzimidazol-2-yl]-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]ethyl]-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-75-2P, N-{[15]-1-(5-Chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-77-4P, N-{(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-79-6P, N-{[15]-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-{[15]-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-83-2P, N-{[15]-1-(1H-Benzimidazol-2-yl)-

2-[3-chloro-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)pheny)]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-85-47, N-[(15)-1-(1H-Benzimidazol-2-yl)pheny]]ethyl]-3, 4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-69, N-[(15)-1-(1H-Benzimidazol-2-yl)pheny]]ethyl]-3, 4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-69, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-yl)-2-hloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-89-89, 3-chloro-H-(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-91-29, N-[(15)-1-(5-chloro-1H-

benzimidazol-2-yl)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl)-3-fluorobenzenesulfonamide trifluoroacetate

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) disorders, including, for example, diabetes and obesity, that are connected directly or indirectly to the activity of the target protein. Methods of prepn. are claimed and hundreds of example prepns. are included. For example, V was prepd. in 12 steps (50, 62, 100, 59, not detd., 100, 100, 99, not detd., not detd., 43, and 25 % yield) starting from N-tert-butyl-3-(2-(tert-buty)carbamoyl)ethyldisultanyl)propionamide. For I-IV: a dashed line indicates an optional bond: Scl is a lst mol. scaffold or is absent; Sc2 is a 2nd mol. scaffold or is absent, wherein

least one of Sc1 and Sc2 is present; or Sc1 and Sc2 together with X1 and X2 or X4 and X5 form a 5-, 6-, or 7-membered fused carbocyclic ring or a 5-, 6-, or 7-membered fused heterocarbocyclic ring; X1 is C or N when Sc1 is present; X1 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc1 is absent, X2 is C or N when Sc2 is present; X2 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2, wherein the ring formed by X1, X2, X3, D1, D2, and D3 is an arom. ring; X4 is C or N when Sc1 is present; X4 is O, S, CR3, N, NR4,

CS, SO, or SO2 when Sc1 is absent; X5 is C or N when Sc2 is present; X5

O, S. CR3, N, NR4, CO, CS, SO, or SO2 when Sc2 is absent; X6 is C or N. Each E1 and E2 = O, S. CR3, N, NR4, CO, CS, SO, or SO2, wherein the ring formed by X4, X5, X6, E1, and E2 is an arom. ring; Rr is H, halo, C1-C4 alky1, C3-C6 cycloalky1, haloalky1, OR28, SR28, NO2, CN, SOR29, SORR9, COR30, COROR31, NR32R31, a 5- or 6-membered heterocarbocycly1 group, or tetraroly1. R15 is H, halo, C1-C4 alky1, C3-C6 cycloalky1, haloalky1,

C1-C4 haloalkyl), SO2(C3-C6 cycloalkyl), SO2NHZ, CHO, COOH, CO(C1-C4 alkyl), CO(C3-C6 cycloalkyl), CO(C1-C4 haloalkyl), CO(heterocarbocyclyl), COO(C1-C4 alkyl), COO(C3-C6 cycloalkyl), COO(C1-C4 haloalkyl), CONHC1-C5 alkyl), CON(C1-C4 alkyl)Z, CONHC1-C5 alkyl)Z, CON(C1-C4 alkyl)Z, CONHC1-C5 cycloalkyl), CON(C3-C6 cycloalkyl), NH(C1-C4 alkyl)Z, NH(C3-C6 cycloalkyl)Z, NH(C1-C4 alkyl)Z, NH(C3-C6 cycloalkyl)Z, NH(C

cycloalkyl) cycloalkyl); or Rl6 and Rl7 together with the C atom to which they are attached form a C3-C6 cycloalkyl group or a 3-7 membered heterocycloalkyl group; and ql is 1 or 2; addnl. details are given in the

Claims.

850315-19-49. [(15)-1-[(15)-1-(Pentylcarbamoyl)-2-[4-[1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]ethyl]carbamoyl)-2-phenylethyl]carbamoyl acid tert-butyl ester 850315-22-9P, [25]-2-[(25)-2-[(2-(4-Wethoxyphenyl)actyl)amino]-3-

phenylpropionyl}amino]-N-pentyl-3-{4-(1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenylpropionamide 850315-24-1P, N-{(1S)-2-{4-(1,1-Dioxido-4-

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 850327-93-4P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)henyllethyl]-3-chlorobenzenesulfonamide trifluoroacetate 850327-95-6P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyllethyl]-3-fluorobenzenesulfonamide trifluoroacetate RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; prepn. of 1-oxo and 1,1-dioxoisothiazolone and

modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins such as phosphatases that bind phosphorylated peptides and proteins selections of the proteins selection of the proteins selection of the proteins selection of the protein of the protei

Absolute stereochemistry

850315-22-9 RCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-(1,1-dloxido-4-0xo-1,2,5-thiadiarolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-24-1 HCAPLUS [1,1'-Biphenyl]-4-sulfonamide, N-[[1S]-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued) Absolute stereochemistry.

RN 850315-36-5 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl]-4(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-35-4 CMF C25 H19 F6 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide,
N-[(1S)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-43-4 CMF C26 H18 F9 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850315-48-9 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)phenyl]-1-[5-(trifluoromethyl)-lH-benzimidazol-2-yl)ethyl)-2(trifluoromethoxy)-, mono(trifluoroacetate) [9CI] (CA INDEX NAME)

CM 1

CRN 850315-47-8 CMF C25 H19 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN CMF C2 H F3 O2 (Continued)

850315-40-1 HCAPLUS
Benzenesulfonamide, 4-bromo-N-[(1S)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-39-8 CMF C25 H18 Br F6 N5 O6 S2

Absolute stereochemistry.

2

850315-44-5 HCAPLUS

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2 CM

CRN 76-05-1 CMF C2 H F3 O2

850315-63-8 KCAPLUS [1,1'-Biphenyl]-4-sulfonamide, N-{(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-

1,2,5-thiadiazolidin-2-yl)phenyl]-l-[5-(trifluoromethyl)-lH-benzimidazol-2-yl]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-62-7 CMF C30 H23 C1 F3 N5 O5 S2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-65-0 HCAPLUS

Benzenesulfonamide, N-[(15)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazoldidn-2-yl)phenyl}-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-4-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

см 1

CRN 850315-64-9 CMF C25 H18 C1 F6 N5 O5 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-73-0 HCAPLUS
Benzenesulfonamide, N-[(|s]-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-(5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-72-9 CMF C26 H17 C1 F9 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850315-69-4 HCAPLUS
CN Benzenesulfonanide,
4-bromo-N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-68-3 CMF C25 H17 Br C1 F6 N5 O6 S2

Absolute stereochemistry.

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-65-0 HCAPLUS
CN Benzeneaulfonamide,
N-{(!S)-1-{S-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-,
mono(trifluoroacetate) {9CI} (CA INDEX NAME)

CM 1

CRN 850327-64-9 CMF C23 H19 C12 N5 O5 52

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 850327-67-2 HCAPLUS

Benzenesulfonamide,
N-[[(5)-1-[(5)-chloro-]H-benzimidazol-2-yl)-2-[3-chloro4-[(1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl)phenyl]ethyl]-2-cyano-,
monoftrifluoroacetate) [9C] (CA INDEX NAME]

CM 1

CRN 850327-66-1 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-69-4 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-73-0 HCAPLUS
CN Benzenesulfonamide,
N-{(1S)-1-{5-chloro-1H-benzimidazo1-2-y1}-2-{3-chloro-

4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-3,4-dimethoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-72-9 CMF C25 H23 C12 N5 O7 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide.
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl)-4-cyano-,
bono(trifluoroacetate) (9CI) (CA INDEX NAME) CM 1 CRN 850327-68-3 CMF C24 H18 C12 N6 O5 S2 Absolute stereochemistry.

RN 850327-71-8 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-70-7 CMF C29 H23 C12 N5 O6 52

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-75-2 KCAPLUS
CN Benzenesulfonamide,
N-[{1S}-1-{5-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl}-3,5-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-74-1 CMF C25 H23 C12 N5 O5 S2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-77-4 HCAPLUS
Benzenesulfonamide, N-{(15)-1-(1H-benzimidazol-2-yl)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chladiazolidin-2-yl)phenyl]ethyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-76-3 CMF C23 H20 C1 N5 O5 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenesulfonamide, N=[(15]-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-80-9 CMF C24 H19 C1 N6 O5 52

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-83-2 HCAPLUS
Benzenesulfonamide, N-[{15}-1-{1H-benzimidazo1-2-y1}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-y1}phenyl]ethyl}-3-phenoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-82-1 CMF C29 H24 C1 N5 O6 S2

Absolute stereochemistry.

14 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

СМ 2

F-C-C02H

RN 850327-79-6 HCAPLUS
CN Benzenesulfonanide, N-{(15)-1-{1H-benzimidazo1-2-y1}-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-2-cyano-, mono(trifluoroacetate) | 9CI) | (CA INDEX NAME)

СМ 1

CRN 850327-78-5 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

2 CM

CRN 76-05-1 CMF C2 H F3 O2

CO2H

RN 850327-81-0 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2

CRN 76-05-1 CMF C2 H F3 O2

850327-85-4 HCAPLUS
Benzenesulfonanide, N-[{ls}-1-{lH-benzimidazol-2-yl}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenyl}ethyl}-3,4-dimethoxy-,mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-84-3 CMF C25 H24 C1 N5 O7 52

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850327-87-6 HCAPLUS
Benzenesulfonamide, N-{(1S)-1-(1H-benzimidazol-2-yl)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-3,5-dimethyl-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-86-5 CMF C25 H24 C1 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2 CM

850327-93-4 HCAPLUS
Benzenesulfonamide, N-{{15}-1-{1H-benzimidazol-2-yl}-2-{3-chloro-4-{1,1-dioxido-4-oxe-1,2,5-thiadiazolidin-2-yl]phenyl]ethyl}-3-chloro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 650327-92-3 CMF C23 H19 C12 N5 O5 S2

Absolute stereochemistry.

CM 2

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

850327-89-8 HCAPLUS
Benzenesulfonamide, 3-chloro-N-{[15]-1-(5-chloro-1H-benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl}-, monottrifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-88-7 CMF C23 H18 C13 N5 O5 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-91-2 HCAPLUS
Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-90-1 CMF C23 H18 C12 F N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 76-05-1 CMF C2 H F3 O2

850327-95-6 HCAPLUS
Benzenesulfonamide, N-{(15)-1-(1H-benzimidazol-2-yl)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-94-5 CMF C23 H19 C1 F N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 850315-20-7P, [(S)-2-[4-(5-Benzyl-1,1,4-

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) ester 850315-23-0P, (28)-3-(4-(5-Benzyl-1),1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]-2-{(25)-2-[{2-(4-methoxyphenyl)accey],amino]-3-phenylpropionyl]amino]-N-pentylpropionamide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of 1-0xo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins) 850315-20-7 HCAPLUS Carbamic acid, [(1S)-1-[(4-(1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)-2-oxo-2-(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-21-8 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl)-L-phenylalanyl-4-{1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM

ED Entered STN: 11 Apr 2005
ACCESSION NUMBER: 2005:308290 HCAPLUS
DOCUMENT NUMBER: 143:7658
AUTHOR(S): Expedient syntheses of sulfonylhydantoins and two six-membered analogs and two six-membered analogs
AUTHOR(S): Campbell, Andrew D.; Birch, Alan M.
Research and Development, AstraZeneca, Cheshire, SK10
4TG, UK
SUNCE: SyNLEX; ISSN: 0936-5214
CODEN: SYNLEX; ISSN: 0936-5214
CODEN:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

A range of α -amino esters can be turned into sulfonylhydantoins in a single, atom-economic step using sulfamide and DBU. E.g., reaction of BANKCH2CO2E with sulfamide and DBU gave 65% sulfonylhydantoin I. This procedure obviates the need for a three- or four-step sequence utilized

traditional procedures. Two new six-membered analogs [5-aryl-1,2,6-thiadiazinan-3-one 1,1-dioxides and 5-aryl-1,2-thiazinan-3-one 1,1-dioxides), e.g. II and III, have also been prepared utilizing novel synthetic protocols.
612528-23-1P 612529-46-IP 612530-69-5P 852338-50-0P 852338-51-1P 852358-53-3P 852388-54-4P 852358-56-98 852388-57-7P RL: SPN (Synthetic preparation); PREP (Preparation)

(Continued) L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (prepn. of sulfonylhydantoins via reaction of amino acid esters with sulfamide and DBU) 612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) [CAINDEX NAME]

612529-46-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-bromophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

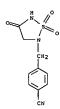
RN 852358-50-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-, 1,1-dioxide
(9C1)

(CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-51-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2-methoxyphenyl)methyl]-, 1,1-dioxide (951) (CA INDEX NAME)

852358-53-3 HCAPLUS Benzonitrile, 4-{(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl}-(9C1) (CA IMDEX NAME)



852358-54-4 HCAPLUS

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN



THERE ARE 20 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: 20 RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
ethyl ester (9CI) (CA INDEX NAME)

852358-56-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{1,1'-biphenyl}-3-ylmethyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

852358-57-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-methyl-5-(phenylmethyl)-, 1,1-dioxide, (45) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 08 Mar 2005 ACCESSION NUMBER: 2005:202894 HCAPLUS DOCUMENT NUMBER: 142:366767

1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides are potent inhibitors of human TITLE:

AUTHOR (5):

heterocyclic sulfides are potent inhibitors of hum tryptase
Wong, Tzutshin; Groutas, Christopher S.; Mohan, Swathi; Lai, Zhong; Alliston, Kevin R.; Vu, Nga; Schechter, Norman M.; Groutas, William C. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Archives of Biochemistry and Biophysics (2005), 436(1), 1-7 CODEN: ABBIA4; ISSN: 0003-9861

CORPORATE SOURCE:

SOURCE:

Elsevier

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors describe herein the design, synthesis, and in vitro biochem.
evaluation of a series of potent, time-dependent inhibitors of the mast
cell-derived serine protease tryptase. The inhibitors were readily
obtained by attaching various heterocyclic thiols, as well as a basic
primary specificity residue P1, to the 1,2,5-thiadiazolidin-3-one
1,1-dioxide scaffold. The inhibitors were found to be devoid of any
inhibitory activity toward a neutral (elastase) or cysteine (papain)
protease, however they were also fairly efficient inhibitors of bovine
trypsin. The differential inhibition observed with trypsin suggests that
enzyme selectivity can be optimized by exploiting differences in the S'
subsites of the two enzymes. The results described herein demonstrate
the

versatility of the heterocyclic scaffold in fashioning mechanism-based inhibitors of neutral, basic, and acidic (chymo)trypsin-like serine

inhibitors or neutral, december of the proteases.

849415-30-1P 849415-31-2P 849415-32-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(1,2,5-Thiadiazolidin-3-one l,1-dioxide-based heterocyclic sulfides

potent inhibitors of human tryptase)
849415-30-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{4-aminobutyl}-2-[(2-benzoxazolylthio)methyl}-5-(phenylmethyl)-, 1,1-dioxide, (45)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

849415-32-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-(((3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX INMEX)

Absolute stereochemistry.

849415-24-3P 849415-25-4P 849415-26-5P 849415-27-6P 849415-28-7P 849415-29-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

potent inhibitors of human tryptase)
849415-24-3 RCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-1,2,5thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

are

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

849415-28-7 HCAPLUS
Carbamic acid, [4-[{35}-1,1-dioxido-4-oxo-2-{phenylmethyl}-5-[{{5-phenyl-1,3,4-oxadiazol-2-yl}thio|methyl}-1,2,5-thiadiazolidin-3-yl}butyl}-,
phenylmethyl ester [9CI] (CA INDEX NAME)

Absolute stereochemistry.

849415-29-8 MCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-{phenylmethyl}-5-[[(3-phenyl-1,2,4-oxadiazol-5-y)]thio]methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

849415-25-4 HCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-3-yl]butyl)-, phenylmethyl ester

(9CI) (CA INDEX NAME) Absolute stereochemistry.

849415-26-5 HCAPLUS
Carbamic acid, [4-[(3S)-5-{chloromethyl}-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 849415-27-6 HCAPLUS
CN Carbamic acid,
[4-{(35)-5-{(2-benzoxazolylthio)methyl}-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl}butyl}-, phenylmethyl ester
(SCI)

(CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR
THIS

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 Aug 2004
ACCESSION NUMBER: 2004:677210 HCAPLUS
DOCUMENT NUMBER: 141:235669
Potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin-3-one 1,1 dioxide-based
sulfonamide derivatives
Lai, Zhong; Gan, Xiangdong; Wei, Liuqing; Alliston,
Kevin R.; Yu, Hongyir Li, Yue H.; Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Archives of Biochemistry and Biophysics (2004),
429(2), 191-197
CODEN: ABBIA4; ISSN: 0003-9861
Elsevier
DOCUMENT TYPE: Journal

DOCUMENT TYPE: Journal LANGUAGE:

English CASREACT 141:235669 OTHER SOURCE(S):

R SOURCE(S): CASREAUT 141:235669
The design, synthesis, and in vitro biochem. evaluation of a class of mechanism-based inhibitors of human leukocyte elastase (MLE) that incorporate in their structure a 1,2,5-thladiazolidin-3-one 1,1-dioxide scaffold with appropriate recognition and reactivity elements appended to it is described. The synthesized compds. were found to be efficient, time-dependent inhibitors of HLE. The interaction of the inhibitors with HLE is postulated to lead to the formation of a highly reactive ltonyl

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 212331-99-2P 749866-30-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
RN 212331-99-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

749866-30-6 HCAPLUS Ethanethioic acid, S-[[[45]-4-[2-methylpropy]]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester [9CI] (CA INDEX NAME)

Absolute stereochemistry.

IT 220869-64-7
RL: RCT (Reactant): RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
RN 220869-64-7 RCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

1.4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS On STN (Continued)

749866-32-8 HCAPLUS
D-Phenylalanine, N-[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-33-9 HCAPLUS
L-Phenylalanine, N-{[[(4S)-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}sulfonyl}-, phenylmethyl ester [9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-34-0 HCAPLUS
L-Phenylalanine, N-[{[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

REFERENCE COUNT: THIS

FORMAT

THERE ARE 36 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 30 Jul 2004 ACCESSION NUMBER: 2004:610081 HCAPLUS DOCUMENT NUMBER: 141:157120 Preparation of Title: 141:157120
Preparation of sulfahydantoins as phosphate isosteres for use as phosphatase inhibitors in the treatment of cancer and autoimpune disorders
Saunders, Jeffrey O.: Mikhis, Gregory F.: Blake,

INVENTOR(S): James

PATENT ASSIGNEE(5):

r. Vertex Pharmaceuticals Incorporated, USA PCT Int. Appl., 62 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT	NO.	K	CIND	DATE	APPLIC.	ATION NO.	DATE
	WO 200	4062664		A1	20040729	WO 200	3-US41630	20031230
	W:	AE, AG,	AL, A	M, AT	AU, AZ,	BA, BB, B	G, BR, BY,	BZ, CA, CH, CN,
		CO, CR,	cu, c	Z, DE	, DK, DM,	DZ, EC, E	E, ES, FI,	GB, GD, GE, GH,
		GM. HR.	HU. I	D, IL	IN, 15,	JP, KE, K	G, KP, KR,	KZ, LC, LK, LR,
								NO, NZ, OM, PH,
								TR, TT, T2, UA,
						ZW .		
	DW							ZM, ZW, AM, AZ,
		BY KG.	KZ. M	ID. RU	TJ. TM.	AT. BE. B	G, CH, CY,	CZ, DE, DK, EE,
		ES FI	FR. G	B. GR	HU. IE.	IT. LU. M	C. NL. PT.	RO, SE, SI, SK,
		TR RF	BJ. C	F. CG	CI. CM.	GA. GN. G	D. GW. ML.	MR, NE, SN, TD,
TG		111, 21,		,	,,,	,		
10	CB 251	1818		A 1	20040729	CA 200	3-2511818	20031230
	AII 200	3300447		A I	20040810	AU 200	3-300447	20031230
	110 200	4167187		A 1	20040826	US 200	3-749121	20031230
	PD 150	4407		A 1	20051116	EP 200	3-815258	20031230
	EP 139	1121 DT BP	CH F	אי טא	FS FD	GB GR T	T. LT. LU.	NL, SE, MC, PT,
	κ.	AI, BE,	TT I	V ET	, DO, MK	CV AL T	R BG CZ.	EE, HU, SK
		(5) 40(0	D1, 1	,,	20060618	TR 200	4-566641	20031230
	JP 200	6514960			20000310	115 200	2-4375720	P 20021230
PRIC	DRITY AP	PLN. INFO	,. :			US 200	4 79/3/25	. 10021230
						WO 200	3_11641630	W 20031230
						#O 200	7-0241030	# 20031230

OTHER SOURCE(5): MARPAT 141:157120

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 4-(1.1,4-Trioxo-[1.2,5]thiadiazolidin-2-yl)benzoic acid methyl ester 729600-47-9P 729600-48-0P 729600-49-1P 729600-50-4P 129600-51-5P 729600-52-6P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapoutic use); BIOL (Biological study); PREP (Preparation); USES (Uses

(prepn. of sulfahydantoins as phosphate isosteres for use as protein or phosphatase inhibitors in treatment of cancer and autoimmune

disorders)
RN 612527-99-8 HCAPLUS
CN Benzoic acid, 4-(11,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yi)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-44-6 HCAPLUS Benzoic acid, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-, methyl cater (9C1) (CA INDEX NAME)

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

The invention relates to compds. having a sulfahydantoin or a reverse sulfahydantoin moiety (I) and (II) or pharmaceutically acceptable salts thereof (Q = each (un)substituted C1-8 aliphatic group, C6-10 aryl, heteroaryl having 3-10 ring atoms, heterocyclyl having 3-10 ring atoms; T = C1-6 alkylidene chain wherein one or two nonadjacent methylene units of T are optionally and independently replaced by O, NR, S, CO, CONR, NRCO, NRCONR, SO, SOZ, NRSOZ, SOZNR, or NRSOZNR; m = 0.1; X = CH2, CO, CF2: R = H or (un)substituted C1-8 aliphatic group or two R groups bound to the

(Continued)

nitrogen are taken together with the nitrogen to form a 3-7 membered heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen,

heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen, ein control to the compact and the control to the contro

proliferative disease is selected from acute myelogenous leukemia, chronic

Nelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple
myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple
myelogenous and HTV-1-mediated tumorigenesis. The angiogenic disorder is
selected from solid tumors, ocular neovasculization, and infantile
heansionans. The cancer is selected from colon, breast, stomach, and
vorth cancer. Thus, N-alkylation of Ne 4-aminobenzoate by Et
promoacetate in the presence of Et3N at 60' for 2.5 days gave
4-[(Ethoxycarbonyl)methyl]amino|benzoic acid Me ester which underwent
N-sulfamoylation by sulfamoyl chloride in the presence of Et3N in CH3C12
at room temperature overnight to give 4-[N-[(Ethoxycarbonyl)methyl]-Nsulfamoylamino|benzoic acid Me ester (III). Cyclization of III by
treatment atth NaOMe/MeON at room temperature overnight gave
4-[1,1,4-trioxo-1,2,5-chiadiszolidin-2-yl]benzoic acid Me ester [IV]. IV
showed ICSO of 1.0-100 MM against protein tyrosine phosphatase SHP-2.
IT 612527-99-8P 612530-69-5P 729600-44-6P,

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

729600-47-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-48-0 HCAPLUS
Benzoic acid, 3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, methyl ester (9C1) (CA INDEX NAME)

729600-49-1 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 5-(3-phenyl-2-propenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2-CH=CH-Ph

729600-50-4 HCAPLUS Benzamida, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

NH- (CH2) 4-Ph

729600-51-5 HCAPLUS
Benzamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

NH-- CH2- Ph

729600-52-6 HCAPLUS
Benzamide, N-butyl-4-(1,1-dioxide-4-oxe-1,2,5-thiadiazolidin-2-yl)- {9CI}
(CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 23 Jul 2004 ACCESSION NUMBER: 2004:589375 HCAPLUS DOCUMENT NUMBER: 141:140459

141:140459
Preparation of sulfamides as anti-cancer agents
Plynn, Daniel L.: Petrillo, Peter A.
Deciphera Pharmaceuticals, Inc., USA
PCT Int. Appl., 168 pp.
CODEN: PIXXD2 INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

Patent

English

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

DATE APPLICATION NO. PATENT NO. KIND DATE A2 A3 20040722 WO 2003-US41425 20031226 WO 2004060305 2004060305 A3 20050210
W: AE, AG, AL, AM, AT, AU, AE, BA, BB, BG, BR, BY, B2, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, M2, NO, NZ, CM, PH, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, V1, V2A, ZM, ZW
RW: BW, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BT, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, HR, NE, SN, TD, WO 2004060305 US 2004171075 A1 20040902 US 2003-146545 20031224
US 2004176395 A1 20040909 US 2003-746607 20031224
CA 2511840 A1 20040909 US 2003-746607 20031225
AU 2003303639 A1 20040722 A2 2003-2511840 20031226
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, TT, LI, LU, NL, SE, MC, PT, CS, TE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
ER 200317863 A 20051005 BR 2003-17861 20031226
CN 1756849 A 20060405 CN 2003-80110049 20031226
CN 1791596 A 20060405 CN 2003-80110049 20031226
CN 1791596 T 20060821 UN 2003-80110049 20031226
ERITY APPLN. INFO:: US 2002-437304P P 20021231 TG CN 1756849 CN 1791596 JP 2006519765 PRIORITY APPLN. INFO.: US 2002-437403P P 20021231 US 2002-437415P P 20021231 US 2002-437487P US 2003-463804P P 20030418 US 2003-746545 A 20031224 US 2003-746607 A 20031224 WO 2003-US41425 W 20031226

OTHER SOURCE(S): MARPAT 141:140459 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Sulfamides, such as I, were prepared for use as anticancer agents which

by modulating the activation states of abl or bcr-abl α-kinase proteins. Thus, 4-H02CC6H4CH2NHSOZNHCOR [R = pyrrolidino], prepared from 4-Me02CC6H4CH2NH2 and pyrrolidine, was treated with the pyrimidinylaminoaniline fragment to give I, which showed 10% inhibition

non-phosphorylated abl kinase at 10µM.
726192-44-5P 726192-45-6P 726192-60-5P
726192-61-6P
RL: PRC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of sulfamides as anti-cancer agents)
726192-44-5 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl)amino]phenyl)- (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4methyl-3-{(4-phenyl-2-pyrimidinyl)amino)phenyl]- (9C1) (CA INDEX NAME)

726192-60-5 HCAPLUS
Benzamide, 4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl]-N-[4-methyl-3-(2-pyrimidinylamino)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612527-99-8P 612528-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfamides as anti-cancer agents)
612527-99-8 HCAPLUS
Benzoic acid, 4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-,
methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

726192-61-6 HCAPLUS Urea, N-[4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-N'-[4-methyl-3-(2-pyrimidinylamino)phenyl]- [9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-00-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 NCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 18 JUN 2004

ACCESSION NUMBER: 2004:493693 HCAPLUS

DOCUMENT NUMBER: 141:54348

Freparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as inhibitors of protein tyrosine phosphatase 1B

Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin

Astraceneca AB, Swed.; Astraceneca UK Limited

FOT Int. Appl., 48 pp.

CODDN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

***************************************						KIND DATE				APPLICATION NO.						DATE		
WO 2004050646					A1			20040617		WO 2003-GB5120					20031126			
	W:	AE.	AG.	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		co.	CR.	cυ,	CZ,	DE,	DK,	DM,	D2,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GE,	
		GH.	GM.	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	
		LR,	LS,	LŤ,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NI,	NO,	NZ.	
		OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	sκ,	SL,	SY,	ΤJ,	TM.	
		TN.	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	vc,	VN,	Yυ,	ZA,	ZM,	ZW			
	RW:	BW.	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	υG,	ZM,	ZW,	AM,	ΑZ	
		BY.	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE	
		ES.	FI.	FR.	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	51,	SK	
		TR.	BF.	BJ.	CF.	CG.	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD	

20040623 AU 2003-302626 GB 2002-27813 AU 2003302626 PRIORITY APPLN. INFO.: A1

WO 2003-GB5120

OTHER SOURCE(S):

MARPAT 141:54348

Title compds. I [wherein Rl = H, (halogeno)alkyl, (hydroxy)alkoxy, alkylamino, etc.; R2 = H, (halogeno)alkyl, halogeno, alkoxy; R3 = alkylamido or (un)substituted alkyl; R4 = H, alkyl, (hetero)aryl; R5 = H

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue Acetamide, N-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methoxyphenyl]methyl]- (9CI) (CA INDEX NAME) (Continued)

705256-61-7 HCAPLUS Butanamide, N-[{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)- (9CI) (CA INDEX NAME)

705256-67-3 HCAPLUS
Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-N-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) or alkyl; and pharmaceutically acceptable salts thereof] were prepd. as inhibitors of protein tyrosine phosphatase 1B (PTB1B). For example, 5-(4-(acctamidomethyl)-1-methoxyphenyl]-1,2,5-thiadiazolidin-3-one 1,1-dioxide (II) was given in multi-step synthesis starting from 3-methoxy-4-nitrobenyl alc. II showed inhibition of human PTB1B with ICSO value of 44pM. Thus, I and their pharmaceutical compns. are useful as inhibitors of protein tyrosine phosphatase 1B for the treatment of diabetes mellitus.

1T 705256-50-4P 705256-54-BP 705256-55-9P 705256-61-P7 05256-61-P 705256-61-P 705256-61-P 705256-61-P 705256-61-P 705256-61-P 705256-78-P 705256-7

(Uses)
(preparation of S-phenyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide derivs. as:
inhibitors of protein tyrosine phosphatase 1B)
RN 705256-50-4 RCAPCIUS
CN Accetamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-54-8 HCAPLUS Benzeneacetonitrile, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(951) (CA INDEX NAME)

705256-55-9 HCAPLUS

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 705256-72-0 HCAPLUS Benzenspentanamide, N-[(4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-78-6 HCAPLUS Acetamide, Nr. [[4-(3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-82-2 HCAPLUS
Acetamide, N-[2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]- [9CI] (CA INDEX NAME)

AcNH-CH2

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) alkoxy, C1-6 alkoxy-C1-6 alkoxy, aryloxy, aryl-c1-6 alkoxy, aryloxy-C1-6 alkoxy, heteroaryl-C1-6 alkoxy, heteroaryloxy-C1-6 alkoxy, C1-6 alkoxy-C1-6 alkoxy-C1-6

they are attached form a 5-7 membered carbocyclic or heterocyclic ring;

and R4 are selected such that (i) R3 = hydrogen, C1-6 alkyl, C1-6 alkyl, C1-6 alkylthio or halo and R4 = aryl, biaryl, heteroaryl, C2-6 alkynyl, C3-7 cycloalkyl, arylcarbonyl, heteroarylcarbonyl, aryl-C2-6 alkynyl, aryl-C2-6 alkynyl, c1-6 alkoxy, C1-6 alkylthio, or hateroaryl-C2-6 alkenyl or (ii) R4 = H, C1-6 alkyl, c2-6 alkynyl, C1-7 cycloalkyl, arylcarbonyl, heteroaryl, c2-6 alkynyl, C1-7 cycloalkyl, arylcarbonyl, heteroaryl, c2-6 alkynyl, C1-7 cycloalkyl, arylcarbonyl, heteroarylcarbonyl,

alkenyl, aryl-c2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6

alkenyl, aryl-c2-6 alkynyl or heteroaryl-c2-6 alkenyl; R5 = H, C1-6
alkyl,
C1-6 alkoxy, C1-6 alkylthio, halo-c1-6 alkyl, halo; R6 = H, C1-6 alkyl;
Wherein any aryl, biaryl or heteroaryl group is optionally substituted]
are prepd. These compds are useful as inhibitors of protein tyrosine
phosphatase PTP1B for the treatment of diabetes mellitus. Thus,
4-tolylboronic acid was coupled with 5-(4-bromophenyl)-1,2,5thiadiazolidin-3-one in the presence of
tetrakis(triphenylphosphine)pallad
ium(0) [Pd(PPh]4) and cesium carbonate in a mixt. of DMF, DME, EtOH, and
H2O at 170' for 600 s to give 5-(4'-Methyl-1,1'-biphenyl-4-yl)1,2,5-thiadiazolidin-3-one 1,1-doxide.

IT 692765-08-5P 692765-17-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of phenylthiadiazolidinones as inhibitors of protein
tyrosine
phosphatase 1B (FTP1B) for treatment of diabetes mellitus)

phosphatase 1B (PTP1B) for treatment of diabetes mellitus) 692765-08-5 HCAPLUS [1,1'-Bipheny]-4-carboxylic acid, 3'-[1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

692765-17-6 HCAPLUS [1,1'-Biphenyl]-1-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 21 May 2004 ACCESSION NUMBER: 2004:412929 HCAPLUS DOCUMENT NUMBER: 140:423678 Preparation of 5-(substituted Propagation of 5-(substituted Propagati

phenyl)thiadiazolidin-3-

ones as inhibitors of protein tyrosine phosphatase 1B Birch, Alam Martin; Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 89 pp. CODEN: PIXXD2 INVENTOR(S): PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

PA	PATENT NO.					KIND DATE												
WO	2004	0417	99		A1		2004	0521	1	WO 2	003-	GB47:	21		2	0031	103	
	W:	AE,	AG,	AL,	AM.	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		co.	CR.	CU.	cz.	DE.	DK,	DM,	DZ,	EC,	£E,	EG,	ES,	FI,	GB,	GD,	GE,	
		GH.	GM.	HR.	HU.	ID.	IL.	IN,	IS,	JP,	KE,	KG,	KΡ,	KR,	ΚZ,	LC,	LK,	
									MG,									
		OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	5Υ,	TJ,	TM,	
		TN.	TR,	TT,	TZ,	UA,	UG.	US,	UZ,	vc,	VN,	YU,	ZA,	ZM,	ZW			
	RW:	BW,	GH,	GM,	KE.	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	Z₩,	AM,	AZ,	
		BY,	KG,	KZ,	MD.	RU,	TJ.	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DΚ,	EE,	
		ES.	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	
		TR.	BF.	BJ.	CF.	CG.	CI.	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	

AU 2003278392 PRIORITY APPLN. INFO.: GB 2002-25986 A 20021107

WO 2003-GB4721 w 20031103

OTHER SOURCE(S):

MARPAT 140:423678

AB The title compds. (I) or pharmaceutically acceptable salts thereof [Rl = H, halo, Cl-6 alkyl, Cl-6 alkoxy, Cl-6 alkylthio, halo-Cl-6 alkyl, halo-Cl-6 alkoxy, halo-Cl-6 alkylthio, hydroxy-Cl-6 alkoxy, dihydroxy-Cl-6

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CO2H

692764-76-4P 692764-77-5P 692764-78-6P
692764-79-7P 692764-80-0P 692764-81-1P
692764-82-2P 692764-80-3P 692764-81-4P
692764-92-5P 692764-80-3P 692764-87-4P
692764-91-3P 692764-80-3P 692764-87-4P
692764-91-3P 692764-89-3P 692764-93-5P
692764-91-3P 692764-98-4P 692764-93-5P
692764-91-3P 692764-98-0P 692764-93-1P
692764-91-3P 692764-98-0P 692764-93-1P
692765-00-7P 692765-01-8P 692765-02-3P
692765-00-7P 692765-01-4P 692765-03-2P
692765-10-3P 692765-11-0P 692765-03-2P
692765-10-3P 692765-11-0P 692765-12-1P
692765-13-2P 692765-11-0P 692765-13-4P
692765-13-2P 692765-14-3P 692765-13-4P
692765-20-1P 692765-13-4P 692765-13-4P
692765-30-3P 692765-31-4P 692765-13-4P
692765-30-3P 692765-31-4P 692765-31-4P
692765-31-8P 692765-31-6P 692765-31-4P
692765-31-8P 692765-31-6P 692765-31-4P
692765-31-8P 692765-31-6P 692765-31-4P
692765-31-4P 692765-31-6P 692765-31-4P
692765-31-4P 692765-31-6P 692765-31-4P
692765-31-6P 692765-31-6P 692765-31-4P
692765-30-1P 692765-31-4P 692765-51-6P
692765-30-1P 692765-31-4P 692765-51-6P
692765-30-1P 692765-31-4P 692765-51-6P
692765-30-1P 692765-31-4P 692765-51-6P
692765-30-1P 692765-61-3P 692765-51-6P
692765-31-4P 692765-61-69-9P 692765-51-6P
692765-31-4P 692765-61-69-9P 692765-51-4P
692765-31-4P 692765-51-4P 692765-51-4P
692765-71-4P 692765-51-4P 692765-51-4P
692765-71-4P 692765-51-4P 692765-51-4P
692765-71-4P 692765-51-4P 692765-51-4P
692765 (preparation of phenylthiadiazolidinones as inhibitors of protein

tyrosine

phosphatase lB (PTPlB) for treatment of diabetes mellitus)
692764-76-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-4-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-77-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-nitro[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-78-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-dichloro[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-81-1 HCAPLUS
CN Acetamide, N-{4'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1){1,1'-biphenyl}-3-y1}- (9CI) (CA INDEX NAME)

RN 692764-82-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-83-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl{1,1'-biphenyl}-3-yl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-79-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-80-0 HCAPLUS
CN 1,2,5-Thiaddazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (951) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 692764-84-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(methylthio){1,1'-biphenyl}-3-yl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692764-85-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl(1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9c1) (CA INDEX NAME)

RN 692764-86-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-87-7 HCAPLUS Acetamide, N-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl) $\{1,1'-biphenyl]$ -3-yl]- (GC1 NDEX NAME)

692764-88-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[3-(2-benzofuranyl)phenyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

692764-89-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692764-93-5 HCAPLUS 1,2,5-Thiadiacalidin-3-one, 5-{1,1'-biphenyl}-4-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

692764-94-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CR INDEX NAME)

692764-95-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-90-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{3-{5-oxazolyl}phenyl}-, 1,1-dioxide {9CI}
(CA INDEX NAME)

692764-91-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(4-cyclohexylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692764-92-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-benzoylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-96-8 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 5-(4,4'-dimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-97-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-4'-phenoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-98-0 HCAPLUS CN [1,1"-Biphenyl]-3-carbonitrile, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-99-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-nitro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-00-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4-dimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-01-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-hydroxy-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-05-2 HCAPLUS
CN Acetamide, N-[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-4'methoxy[1,1'-biphenyl]-3-yl]- (9CI) (CA INDEX NAME)

RN 692765-06-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-07-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-acetyl-4-methoxy(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-02-9 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-(3',4,4'-trimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-4'-(trifluoromethyl){1,1'-biphenyl)-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-04-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{5-{1,3-benzodioxol-5-yl}-2-methoxyphenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

RN 692765-09-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1E)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-10-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(2-naphthalenyl)phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4'-(hydroxymethyl)-4-methoxy[1,1'-biphenyl)-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-12-1 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-[4-methoxy-3'-(methoxymethyl){1,1'-biphenyl}-3-yl]-,1,1-dioxide (9CI) (CA INDEX NAME)

MeO.

RN 692765-13-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

0 HeO O-CH2-Ph

RN 692765-14-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-4'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

MeO CH2-OMe

RN 692765-19-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(nethylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

MeO Neo

RN 692765-20-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

H O N S O

RN 692765-21-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy(1,1'-bipheny1)-3-y1)-, 1,1-dioxide (921) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO CH2-Ph

RN 692765-15-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(12]-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

H O Ph

RN 692765-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-[{1,1-dimethylethoxy)methyl}-4-methoxy[1,1'-biphenyl]-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

MeO CH2-OBu-t

RN 692765-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO MeO

RN 692765-22-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-difluoro-4-methoxy{1,1'-biphenyl}-3y1)-,1,1-dioxide (9CI) (CA INDEX NAME)

Meo Meo

RN 692765-23-4 HCAPLUS
CN 1,2,5-Thiadiazoliddin-3-one, 5-(5'-fluoro-2',4-dimethoxy{1,1'-biphenyl}-3-yl)-, 1,1-dioxide (9CT) (CA INDEX NAME)

H N OM

RN 692765-24-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, S-(4-methoxy[1,1':3',1''-terphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-25-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(1,1-dimethylethyl)-4-methoxy(1,1'-biphenyl)-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[(1E)-2-(4-chlorophenyl)+ethenyl]-2methoxyphenyl]-1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-33-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-ethenyl-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RM 692765-28-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1':4',1''-terphenyl]-J-yl)-,
1,1-dioxide (921) (CA INDEX NAME)

RN 692765-29-0 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 5-(3'-chloro-4'-fluoro-4-methoxy[1,1'-bipheny]1-3-y1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-30-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1':4',1''-terphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-furanyl)-2-methoxyphenyl]-,
1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-35-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-benzo[b]thien-2-yl-2-methoxyphenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{5-(2-benzofuranyl)-2-methoxyphenyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-37-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-acetyl-4-methoxy(1,1'-biphenyl)-3-yl)-,

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-38-1 HCAPLUS CN (1.1'-Biphenyl)-3-carboxamide, 3'-(1.1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-39-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-(1H-pyrazol-4-yl)phenyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-40-5 HCAPLUS
CN Pyrrolidine, 1-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]carbonyl)- [9C1] (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

RN 692765-44-9 HCAPLUS
CN [1,1"-Biphenyl]-4-carboxamide, N-cyclohexyl-3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-amino-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 692765-46-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(dimethylamino)-4-methoxy(1,1'-biphenyl)-3-yl]-,1,1-dioxide (9C1) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-4]-6 HCAPLUS
CN {1,1'-Biphenyl]-4-propanoic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-42-7 HCAPLUS
CN Carbamic acid, [[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA
INDEX NAME)

RN 692765-43-8 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-47-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(4-pyridinyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-48-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-hydroxy-4-methoxy[1,1'-biphenyl}-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-49-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-(1H-indol-6-yl)-2-methoxyphenyl)-,
1,1-dioxide (8CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-50-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(2-thienyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2-methoxy-5-(phenylethynyl)phenyl]-,
1,1-dioxide (921) (CA INDEX NAME)

RN 692765-52-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[3-phenyl-1-propynyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-56-3 HCAPLUS

Benzoic acid, 2-[2-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]ethoxy]-6-hydroxy-, methyl ester [9CI] (CA
INDEX NAME)

RN 692765-57-4 HCAPLUS
Benzoic acid, 2-[(3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-3-yl]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-58-S HCAPLUS
CN Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny]]-4-y1]methoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-53-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{5-ethynyl-2-methoxyphenyl}-, 1,1-dioxide
(9CI) (CA INDEX NAME) .

RN 692765-54-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methyl[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-55-2 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy(1,1'-biphenyi)-3-y1)ethoxy|-6-hydroxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-59-6 HCAPLUS
Enzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-4-yl]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-60-9 HCAPLUS CN Benzoic acid, 2-[2-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-baphenyl]-4-y1]ethoxy[-6-hydroxy- (9CI) (CA INDEX NAME)

RN 692765-61-0 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphanyl]-4-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-62-1 HCAPLUS
Benzoic acid, 2-{3-{3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-4'-methoxy{1,1'-bipheny1}-3-y1}propoxy}-6-hydroxy- (9CI) (CA INDEX NAME)

692765-63-2 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-64-3 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-4-yl]propoxy]-6-hydroxy-(9C1) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 692765-68-7 HCAPLUS
CN Benzoic acid,
2-[2-1[[3"-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-y1)-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester (9c1) (CA INDEX NAME)

RN 692765-69-8 HCAPLUS
CN Benzoic acid,
2-[3-1[[3]"-[1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl)-4"methoxy[1,1"-blphenyl]-3-yl]carbonyl]amino]propoxy]-6-hydroxy-, methyl
ester (9C1) (CA INDEX MAME)

RN 692765-70-1 HCAPLUS
CN Benzoic acid,
2-{[5-{[[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-4'methoxy[1,1'-biphenyl]-3-y1]carbonyl]amino]pentyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-65-4 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methox[1,1'-biphenyl]-4-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA
HOBZ NAME)

692765-66-5 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methoxy[-6-hydroxy- [9Cl] (CA INDEX NAME)

RN 692765-67-6 HCAPLUS CN [1,1'-Biphenyl]-3-carboxamide, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-mathoxy-N-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-71-2 HCAPLUS
CN Benzoic acid,
2-[[6-[[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]carbony1]amino]hexy1]oxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX NAME)

RN 692765-72-3 HCAPLUS
CN Benzoic acid,
2-{2-{[[[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-4-y1]carbonyl]amino]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-73-4 HCAPLUS
CN Benzoic acid,
2-[3-[([3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]carbonyl]amino[propoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-74-5 HCAPLUS
CN Benzoic acid,
C[S-[[3]*-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]carbonyl]amino]pentyl]oxy]-6-hydroxy-, methyl
cater [9C1] (CA INDEX MANE)

RN 692765-75-6 HCAPLUS
CN Benzoic acid,
2-[[6-[[[3]-(1]-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]carbonyl]amino]hexy1]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

692765-79-0P 692765-80-3P 692765-84-7P
692765-85-8P 692765-86-9P 692766-02-2P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation of phenylthiadiazolidinones as inhibitors of protein

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN methoxyphenyl]- {9CI} (CA INDEX NAME) (Continued)

692765-86-9 HCAPLUS
1,2,5-Thladiazolidin-3-one, 5-[2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-ylphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692766-02-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-iodo-2-methoxyphenyl)-, 1,1-dioxide
(9CI)

(CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
RN 692765-79-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-80-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-84-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(5-bromo-2-methoxyphenyl)-, 1,1-dioxide

(9CI) (CA INDEX NAME)

692765-85-8 HCAPLUS Boronic acid, [3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4-

KIND DATE

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 10 Oct 2003
ACCESSION NUMBER: 2003:796679 HCAPLUS

DOCUMENT NUMBER: 139:307766

TITLE: Preparation of substituted 1,1-dioxo-1,2,5-thiazolidine-3-ones as protein tyrosine phosphatase

and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis Coppola, Gary Mark: Davies, John William: Jewell, Charles Francis, Jr.; Li, Yu-Chin: Wareing, James Richard: Sperbeck, Donald Mark: Stams, Travis Mathew; Topiol, Sidney Wolf: Vlattas, Isidoros Novartis A.-G., Switz: Novartis Pharma G.m.b.H. PCT Int. Appl., 148 pp. CODEN: PIXXD2 Patent English 1

APPLICATION NO.

DATE

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

WO					A1		20031009		WO 2003-EP3466					20030402			
	W:	AE.	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	ΒY,	ΒZ,	CA,	CH,	CN,
		co.	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		HR.	HU.	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KΡ,	KR,	ΚZ,	LC,	LK,	LT,	LU,
		LV.	MA,	MD,	MK,	MN,	MX,	NI,	NO,	NZ,	OM,	PH,	PL,	PT,	RO,	RU,	SC,
		SE.	SG,	SK,	TJ,	TM,	TN,	TR,	TT,	UΑ,	US,	υz,	vc,	VN,	YU,	ZA,	ZW
	RW:	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,
		DK,	EE.	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,
			SK,														
CA	A 2480562				Al	20031009			CA 2003-2480562						20030402		
AU	AU 2003224030				Al	20031013			AU 2003-224030						20030402		
US	2004023974				A1	20040205			US 2003-405728						20030402		
EP	1492780				A1	20050105			EP 2003-720412						20030402		
	R:	AT.	BE.	CH.	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE.	SI.	LT.	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	НU,	SK	
BR	R 2003008974						2005		BR 2003-8974								
	2005090502								US 2003-510026					20030402			
CN	N 1646508				А	20050727			CN 2003-807887					20030402			
	JP 2005535568				20051124			JP 2003-580308					20030402				
	2004						2004	1214	1	NO 2	004-	4745			2	0041	102

CN 2003-807887 JP 2003-580308 NO 2004-4745 US 2002-369779P US 2002-369930P P 20020403

WO 2003-EP3466 W 20030402

OTHER SOURCE(S): MARPAT 139:307766

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Substituted thiazolidinetriones I [L1 = L2 = single bond, O1 = single bond, H, (un)substituted alkyl, cycloalkyl, or aminocarbonyl, carboxy, R1OC(:O), R1OC(:O), R1OS(:O), G2 = O, S, R3N, R, R2 = (un)substituted alkyl, alkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, or aralkylthio, amino, halogen, nitro, carboxy, trifluoromethyl, etc., R1 = (un)substituted alkyl, alkoxy, aralkoxy, aralkyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, aralkyl, alkyl, R1O = (un)substituted alkyl, alkoxycarbonyl, aryl, heteroaryl, aralkyl, heteroaryloxycarbonyl, carbomyl, or sulfonyl; X, Y = CH, N, O, S, R14N, Z = (un)substituted alkyl, alkoxycarbonyl, aryloxycarbonyl, aryloxycarbonyl, carbomyl, or sulfonyl; X, Y = CH, N, O, S, R14N, Z = (un)substituted alkyl, alkoxyalkyl, alkylthioalkyl, alkylaminoalkyl; Z1, Z2, Z3 = CH, N, N(:O), CR1, CR2; R1 and R2 can form an (un)substituted 5 - or 6-membered aromatic or heteroarom. ring; R1 and L1 can form an (un)substituted 5 - or AB

: 7-membered ring interrupted by nitrogen, oxygen or sulfur atoms] such as II are prepared as inhibitors of protein tyrosine phosphatase 1b and

Il protein tyrosine phosphatase for overcoming insulin resistance and modulating glucose levels in the treatment or prevention of metabolic diseases, such as diabetes, or atherosclerosis. II is prepared by

treatment of Et bromoacetate with 1-naphthalenemethanamine, N-sulfamoylation with sulfamoyl chloride, and base-mediated cyclocondensation. No biol. data

is

provided.
612510-89-8P 612530-90-2P 612530-92-4P 612530-93-5P 612530-94-6P 612530-92-4P 612530-93-5P 612530-94-6P 612530-95-7P 612531-00-9P 612531-00-9P 612531-00-9P 612531-01-8P 612531-02-9P 612531-103-9P 612531-103-2P 612531-103-9P 612531-103-6P 612531-60-9P 612531-61-60-612531-63-9P 612531-61-69 612531-66-5P ΙT

(Continued) ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612530-92-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-{(2,4-dimethoxyphenyl)methyl}-5-{(4-methoxy7-quinolinyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-93-5 HCAPLUS

CN Benzoic acid,
4-([5-([2, 4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, [4-(methylthio)phenyl]methyl ester (9CI)
(CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612531-67-6P 612531-68-7P 612531-69-8P
612531-70-1P 612531-71-2P 612531-72-3P
612531-73-4P 612531-75-6P 612531-76-7P
612531-77-8P 612531-78-9P 612531-79-0P
612531-80-3P 612531-78-9P 612531-79-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of thiazolidinetriones as protein tyrosine phosphatase ib and T-cell protein tyrosine phosphatase ib nibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis)
612530-89-9 HCAPLUS
Carbamic acid, [4-{[5-(2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

| OMe

RN 612530-90-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-{{2,4-dimethoxyphenyl}methyl}-5-{{1-ethyl-2-}
methyl-lR-benzimidazol-5-yl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

RN 612530-94-6 HCAPLUS
CN Benzoic acid,
-{{5-{(2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-{thisdiazolidin-2-yl)methyl}-, {4-{methylsulfonyl)phenyl|methyl ester (9CI) (CA INDEX NAME)

RN 612530-95-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{4-{bromomethyl}phenyl}methyl}-2-{(2,4-dimethoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612530-98-0 HCAPLUS

Acetic acid, [[{4-{[5-{(2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-96-8 HCAPLUS
CN Acetic acid, [[[4-[[5-[{2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiacolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612530-99-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-iodophenyl)methyl]-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-00-7 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-01-8 HCAPLUS L-Phenylalanine, N-[{1,1-dimethylethoxy}carbonyl}-3-[$\{5-\{4-1\}\}$]

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}(9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-05-2 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-10-9 HCAPLUS
CN Benzaldehyde,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiediazolidin-2-yl]methyl]- [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-02-9 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[(5-{(4-methoxyphenyl)methyl)-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-2-oxo-2(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-03-0 HCAPLUS Benzenepropanamide, a-amino-3-[[5-[{4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}-N-pentyl-, (a5)-[9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-13-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{2,4-dimethoxyphenyl}methyl}-5-[[4-[{4-(phenylmethyl}-1-piperazinyl]methyl]phenyl]methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

612531-22-3 HCAPLUS
Carbanic acid, [[4-[[5-{[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

PAGE 1-A

612531-23-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612531-30-3 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-[(4-(aminomethyl)phenyl)methyl]-2-[(2,4dimethoxyphenyl)methyl]-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

RN 612531-24-5 HCAPLUS
CN Carbamic acid.
[2-{[4-[5-[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]amino]-2-oxoethyl}-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A RN 612531-31-4 HCAPLUS
CN Benzoic acid,
4-{[5-{[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

RN 612531-32-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[(4-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2

PAGE 1-A

PAGE 2-A

RN 612531-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-(2,4-dinitrophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-35-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-2-[(2,4dimethoxyphenyl)methyl|-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612531-36-9 HCAPLUS
CN Benzoic acid, 3-[5-[[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, methyl ester [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612531-61-0 HCAPLUS
CN 1H-1,4-Benzodiazepine-2,5-dione, 3-{[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-(phenylmethoxy)phenyl)methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)

RN 612531-63-2 HCAPLUS CN 1.2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-2-[(4-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-64-3 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl)-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-,phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-65-4 HCAPLUS CN D-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-68-7 HCAPLUS
CN Benzenepropananide, α-amino-4-[5-[(4-methoxyphenyl]methyl]-1,1dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (αS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612531-69-8 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-[5-{(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

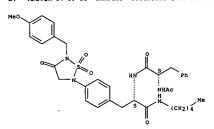
RN 612531-66-5 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-67-6 HCAPLUS
CN Carbamic acid,
[(1S)-1-[[4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1.7,5-thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl}-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 612531-70-1 HCAPLUS
CN L-Phenylalanine, 4-{5-{(4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-71-2 HCAPLUS
CN L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-{(4-methoxyphenyl)methyl)1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl}-, phenylmethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 612531-72-3 HCAPLUS
L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-[(4-methoxyphenyl)methyl]1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-73-4 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-[2-(1,1-dimeth)]+2-0xoethyl]phenyl]ethyl]-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-77-8 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[5-[(4-methoxyphenyl)]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-78-9 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-3-{5-{4-methoxyphenyl|methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-75-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-76-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(3-iodophenyl)-2-(14-methoxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Con

RN 612531-79-0 HCAPLUS CN Carbamic acid, [(15)-1-[[3-[5-[4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phonyl]methyl]-2-oxo-2-[pentylamino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-80-3 HCAPLUS
CN Benzenepropanamide, α-amino-3-[5-[(4-methoxyphenyl)methyl]-1,1dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (αS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

612534-94-8 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

612527-93-2P 612530-46-8P 612530-49-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (invention compound; preparation of thiazolidinetriones as protein

sine phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis) 612527-93-2 HCAPLUS 1,2,5-Thadiazolidin-3-one, 5-[(3-aminophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 612527-98-TP 612520-02-P6 612528-00-4P 612528-01-F9 612528-01-F9 612528-02-P6 612528-01-F9 612528-01-F9 612528-01-F9 612528-01-F9 612528-01-P7 612528-12-P6 612528-13-P9 612528-13-P9 612528-13-P9 612528-13-P9 612528-13-P9 612528-13-P9 612528-14-P6 612528-13-P9 612528-13-P9 612528-14-P6 612528-13-P9 612528-14-P6 612528-13-P9 612528-23-P9 612528-23-P9 612528-23-P9 612528-23-P7 612528-23-P9 612528-23-P9 612528-23-P7 612528-23-P9 612528-23-P7 612528-23-P9 612528-23-P7 612528-23-P9 612528-23-P9 612528-23-P9 612528-23-P9 612528-23-P9 612528-23-P9 612528-24-P9 612528-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-46-8 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
ester (9CI) (CA INDEX NAME)

612530-49-1 HCAPLUS
Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-,
methyl ester (9CI) (CA INDEX NAME)

612527-84-1P 612527-85-2P 612527-86-3P 612527-87-4P 612527-89-6P 612527-90-9P 612527-91-0P 612527-91-0P 612527-91-6P 612527-91-6P 612527-91-6P 612527-91-6P

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612530-04-8P 612530-05-9P 612530-06-0P
612530-08-2P 612530-09-3P 612530-10-6P
612530-11-7P 612530-12-8P 612530-13-9P
612530-16-2P 612530-12-3P 612530-13-9P
612530-29-6P 612530-23-3P 612530-25-3P
612530-22-0P 612530-23-1P 612530-25-3P
612530-29-7P 612530-30-0P 612530-21-1P
612530-32-2P 612530-33-3P 612530-31-1P
612530-39-5P 612530-33-3P 612530-31-4P
612530-38-5P 612530-34-5P
612530-31-3P 612530-31-5P
612530-31-3P 612530-31-5P
612530-44-6P 612530-45-7P 612530-47-9P
612530-48-0P 612530-65-4P 612530-47-9P
612530-48-0P 612530-50-4P 612530-51-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(invention compd.; prepn. of thiazolidinetriones as protein tyrosine phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis)
612527-84-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(1-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-85-2 HCAPLUS
Acetamide, N-(3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y)|methyl|phenyl|methyl|- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN L4

612527-86-3 HCAPLUS
Carbamic acid, [[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, 1,1-dimethylathyl ester (9CI) (CA INDEX NAME)

612527-87-4 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-,: 1,1-dioxide (9C1) (GA INDEX NAME)

612527-88-5 HCAPLUS Acetamide, N-[{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}pheny1}methy1}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-89-6 HCAPLUS
Carbamic acid, [{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612527-90-9 HCAPLUS
Benzenepropanamide, N-{{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}phenyl}methyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612527-91-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(3-iodophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-92-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-nitrophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612527-94-3 HCAPLUS Acetamide, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyll- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN



612527-96-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(4-aminophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued)

612527-97-6 HCAPLUS
Butanamide, N-{3-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}phenyl}- (9CI) (CA INDEX NAME)

RN 612527-98-7 HCAPLUS CN Urea, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-N'-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN propyl- (9CI) (CA INDEX NAME) (Continued)

612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)methyl]-,
methyl ester (9Cl) (CA INDEX NAME)

612528-00-4 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-(9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-07-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-08-2 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[(4-amino-2-bromophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-09-3 HCAPLUS
Acetamide, N-{4-{(1,1-dioxido-4-oxo-1,2,5-thiadia2olidin-2-y1)methy1)pheny1}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-01-5 HCAPLUS
Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-(9CI) (CA INDEX NAME)

RN 612528-02-6 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-{(2-methylphenyl)methyl}-, 1,1-dioxide
(9CI)

(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-10-6 HCAPLUS
Methanesulfonamide, N-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]pheny1}- (9CI) (CA INDEX NAME)

612528-11-7 HCAPLUS
Methanesulfonamide, N-[[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl]phenyl]methyl]- {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)

RN 612520-12-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphenyl)methyl]-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612528-13-9 HCAPLUS
CN Benzeneacetic acid, a-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612528-14-0 HCAPLUS
CN Benzeneacetamide, α-amino-2-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]-N-propy1- (9CI) (CA INDEX NAME)

(Continued)

RN 612528-15-1 HCAPLUS
CN Benzeneacetamide, α-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-16-2 HCAPLUS CN Benzeneacetamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-N-propyl- $\alpha-[\{trifluoroacetyl\}amino]- (9CI) (CA INDEX NAME)$

RN 612528-17-3 HCAPLUS
CN Benzeneacetamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]α-[(methylsulfonyl)amino]-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-18-4 HCAPLUS
CN Benzenepropanamide, a-{acetylamino}-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-19-5 HCAPLUS
CN Propanedioic acid, (acetylamino)[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

RN 612528-20-8 HCAPLUS
CN Benzenepropanmide, a-mmino-4-({1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl)-N-propyl- (9C1) (CA INDEX NAME)

RN 612528-21-9 HCAPLUS
CN Phenylalanine, N-acetyl-4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, ethyl ester (9CI) {CA INDEX NAME}

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-26-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[2-(2-chlorophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAVE)

RN 612528-27-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(4-aminophenyl)ethyl]-, 1,1-dioxide (9C1) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-22-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-α-phenyl-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-23-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-25-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-[3,4-dimethoxyphenyl]ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-28-6 HCAPLUS
CN Acetamide, N-{4-{2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethy1]pheny1}-2,2,2-trifluoro-(9CI) (CA INDEX NAME)

RN 612528-29-7 HCAPLUS
CN Butanamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 612528-32-2 HCAPLUS CN 1,2,5-Thiadiazolidino-2-acetic acid, 4-oxo-α-(phenylmethyl)-, 1,1-dioxide (921) (CA INDEX NAME)

RN 612528-33-3 MCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 5-yl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-37-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((4-methoxy-7-quinolinyl)methyl]-, 1,1-dioxide (901) (CA INDEX NAME)

RN 612528-38-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(2-methylpropoxy)-7-quinolinyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-39-9 HCAPLUS Glycine, N-[2-(butylamino)-2-oxo-1-phenylethyl]-N-[4-{(1,1-dioxido-4-oxo-1,2,5-thiadizolidin-2-yl]methyl]benzoyl- (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-34-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, S-[{4-(aminomethyl)-1-naphthalenyl]methyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-35-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-((1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyll-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-36-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{[2-methyl-1-(3-methylbutyl)-1H-benzimidazol-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-40-2 HCAPLUS Glycine, N-[2-(butylamino)-1-(4-ethylphenyl)-2-oxoethyl]-N-(4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

PAGE 1-A

PAGE 2-A

RN 612528-41-3 HCAPLUS
Glycine, N-[2-(butylamino)-2-oxo-1-(3-phenoxyphenyl)ethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612528-42-4 HCAPLUS
CN 61ycine, N-[2-(butylamino)-1-(4-methoxypheny1)-2-oxocthy1]-N-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]benzoy1]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

Br

NN 612528-44-6 HCAPLUS
Clycine, N-{2-(butylamino)-1-(2-naphthalenyl)-2-oxoethyl)-N-{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}benzoyl}- (9CI) (CA INDEX NAME)

N 612528-45-7 HCAPLUS
N Glycine, N. [12-{butylamino}-1-{4-chloropheny1}-2-oxoethy1}-n-{4-{{1,1-dioxido-4-oxo-1,2,5-chladiazolidin-2-y1}methy1}benzoy1}- [9C1] (CA INDEX

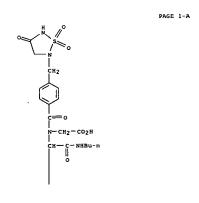
L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612528-43-5 HCAPLUS
CN Glycine, N-[1-(2-bromophenyl)-2-(butylamino)-2-oxoethyl]-N-[4-[(1,1-dioxado-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)



PAGE 2-A

RN 612528-46-8 HCAPLUS
CN Glycine, N-[2-(butylamino)-2-oxo-1-[3-(phenylmethoxy)phenyl)ethyl}-N-[4[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA
INDEX NAME)

PAGE 1-A

PAGE 2-A

\ o-сн₂- Ph

RN 612528-47-9 HCAPLUS
CN Glycine,
N-[(2E)-1-[(butylamino]carbonyl]-3-phenyl-2-propenyl]-N-[4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 612528-48-0 HCAPLUS
CN Glycine,
N-[1-{(butylamino)carbonyl}-3-phenylpropyl}-N-{4-{(1,1-dioxido-4-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) PAGE 2-A

612528-50-4 HCAPLUS
Benzoic acid, 4-((l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(3-chlorophenyl)methyl ester (9C1) (CA INDEX NAME)

PAGE 2-A

612528-51-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, (4-butylphenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-49-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(methylsulfonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 1-A

PAGE 2-A

612528-52-6 HCAPLUS
Benzoic acid, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-,
[4-(hydroxymethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

PAGE 1-A

PAGE 2-A

612528-53-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[2-(2-phenylethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) {4-(difluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

RN 612528-56-0 HCAPLUS
CN 2-Thiopheneacetic acid,
5-[{{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}benzoy1]oxy]methy1}-a,a-difluoro-(9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-54-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[1,1'-biphenyl]-2-ylmethyl ester (9CI) (CA INDEX NAME)

612528-55-9 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-57-1 HCAPLUS Acetic acid, [[[4-[(1,1-dioxido-4-oxo-1,2.5-thiadiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

612528-58-2 HCAPLUS
Acetic acid, [[[4-f(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]]methyl]phenyl]pethyl]thio]-, ethyl ester [901] (CA INDEX NAME)

RN 612528-59-3 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one,
5-{[4-[[d]-methylburyl]thio]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me2CH-CH2-CH2-S-CH2

RN 612528-60-6 HCAPLUS
CN Benzoic acid, 4-(1),1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-ethylbutyl exter (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

RN 612528-64-0 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2,4,4-trimethylpentyl ester (9C1) (CA INDEX NAME)

RN 612528-65-1 HCAPLUS

Senzoic acid, 4-[(1.1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclohoxylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-66-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-62-8 HCAPLUS
CN Benzoic acid, 4-[(l,l-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclopentylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-63-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl}methyl]-,
2-methylpenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-67-3 HCAPLUS

Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclopentyl ester (9CI) (CA INDEX NAME)

RN 612528-68-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2-methylbutyl ester (9C1) (CA IMDEX NAME)

RN 612528-69-5 HCAPLUS
CN Benzoic acid, 4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methylj-,
2-(methylthio)etchyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-70-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-[(carboxymethyl)thio]ethyl ester (9CI) (CA INDEX NAME)

612528-71-9 MCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(5-nitro-2-furanyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-72-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
2-pyridinylmethyl ester (9CI) (CA INDEX NAME)

(Continued)

612528-73-1 HCAPLUS
Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[3-(hydroxymethyl)phenyl]methyl ester (9CT) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

PAGE 1-A

612528-74-2 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[3-(methylsulfonyl)phenyl]methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612528-75-3 HCAPLUS
Benzeneacetic acid, 4-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]amino]butyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

612528-76-4 HCAPLUS
Benzeneacetic acid, 4-[3-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

612528-77-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-[(dimethylamino)methyl]-2-furanyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-78-6 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612528-79-7 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(lH-indol-5-ylmethyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612528-80-0 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[(3,4,5-trimethoxyphenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-82-2 HCAPLUS
1,2,3-Thiadizolidin-3-one, 5-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-83-3 KCAPLUS
Benzeneacetic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (SCI) (CA INDEX NAME)

612528-84-4 HCAPLUS
1.2,5-Thiadiazolidin-3-one, 5-((4-benzoylphenyl)methyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-85-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-86-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{[4-(4-methyl-1-oxopentyl)phenyl]methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

HO2C

RN 612528-89-9 HCAPLUS CN 2(1H)-Quinolinone, 6-[(1,1-dioxido-4-oxo-1,2,5-thiediazolidin-2-y1)methyl]-1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

RN 612528-97-9 HCAPLUS
CN Acetamide, 2-amino-N-{{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}methyl}- (9CI) (CA INDEX NAME)

RN 612528-98-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-carboxyphenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-87-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{{3-{2-fluorophenoxy}phenyl}methyl}-,
1,1-dioxide {9Cl} (CA INDEX NAME)

RN 612528-86-8 HCAPLUS
CN Benzoic acid, 3-{2-{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}ethoxy}- (9CI) (CA INDEX NAME)

PAGE 1-A

H

O

CH2

CH2

CH2

CH2

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612528-99-1 HCAPLUS (3-phenoxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN [Continued] 612529-00-7 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methyl]-3-nitro- (SCI) (CA INDEX NAME)

612529-01-8 HCAPLUS 1,2.5-Thiadiarolidin-3-one, 5-[(4-(hydroxymethyl)phenyl]methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

612529-02-9 HCAPLUS
Benzoic acid, 2-amino-4-((1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-05-2 HCAPLUS
Benzoic acid, 5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yllmethyl)- (9CI) (CA INDEX NAME)

RN 612529-06-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-chloro-3-methoxy-5-nitrophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-03-0 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-{(4-hydroxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-04-1 HCAPLUS Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-5-nitro- [9CI] (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-07-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-08-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-methyl-2-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-09-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-, 1,1-dioxide

(CA INDEX NAME)

RN 612529-10-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-phenylpropyl)-, 1,1-dioxide (9CI) (CA

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) INDEX NAME)

RN 612529-11-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[{4-butoxyphenyl}methyl}-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612529-12-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-13-2 HCAPLUS
CN Benzoic acid, 3-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612529-16-5 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-[(4-methyl-3-nitrophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX MAME)

RN 612529-17-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(5-methyl-2-nitrophenyl)methyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-aminophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-14-3 HCAPLUS
CN Benzenebutanoic acid,
5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]- (9CI) (CA INDEX NAME)

RN 612529-15-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-methyl-3-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-19-0 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin- 2-yl)methyl}phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612529-20-1 RCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[(3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)methyl]phenyl]methyl)- (9C1) (CA INDEX NAME)

RN 612529-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[1,4-phenylenebis(methylene)|bls-,
1,1.1',1'-tetraoxide (9CI) (CA INDEX NAME)

RN 612529-22-3 HCAPLUS CN Acetic acid, [[2-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)methyl]phenyl]anino]oxo- [9CI] (CA INDEX NAME)

RN 612529-23-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-hydroxyphenyl)methyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612529-24-5 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

=-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[{4-fluoro-2-(trifluoromethyl)phenyl}methyl}-, l.-dioxide (9CI) (CA INDEX NAME)

RN 612529-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-28-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (901) (CA INDEX NAME)

RN 612529-29-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-4-methylphenyl)methyl]-,
1,1-dioxide (921) (CA INDEX NAME)

RN 612529-30-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-3-methylphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (



RN 612529-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-2-methylphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-32-5 HCAPLUS
CN 1,2,5-Thiadiasolidin-3-one, 5-((2-amino-5-methylphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-33-6 HCAPLUS CN Acetamide, N-[[4-{[1].dioxido-4-oxo-1,2,5-thiadiazolidin-2yl]medhyl]phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

RN 612529-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3,4-dimethoxyphenyl)methyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612529-37-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-hydroxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612529-41-6 HCAPLUS
CN Benzoic acid, 2-amino-5-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyll-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-42-7 HCAPLUS
EN Benzoic acid,
2-(acetylamino)-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-43-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(phenylmethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-38-1 HCAPLUS 1.2,5-Thiadiazolidin-3-one, 5-[[3,5-dimethylphenyl]methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-39-2 HCAPLUS (13-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl]methyl]-, ethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-40-5 HCAPLUS
CN L-Phenylalanine, N-[[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yi]methyl]phenyl|methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-44-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[{2,4-bis(trifluoromethyl)phenyl]methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,4,6-trifluorophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-46-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-bromophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-47-2 HCAPLUS
1,2,5-Thiadiazolidin-1-one, 5,5'-[[1,1'-biphenyl]-2,2'-diylbis[methylene]|bis-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

612529-48-3 HCAPLUS 1,2.5-Thiadiazolidin-3-one, 5-{{4-{(ethylamino)methyl}phenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-49-4 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Ph-CH2-CH2-NH-

612529-52-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-[(diethylamino)methyl]phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-53-0 HCAPLUS
Benzoic acid, 2-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, phenylmethyl ester {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid,
2-(acetylamino)-4-((1, 1-dioxido-4-oxo-1, 2,5-thiadiazolidin-2-yllmethyl)- (9CI) (CA INDEX NAME)

612529-50-7 HCAPLUS
Benzoic acid, Z-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl|methyl|-, ethyl ester (9CI) (CA INDEX NAME)

RN 612529-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-[(2-phenylethyl)amino|methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-54-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl]methyl}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 612529-56-3 MCAPLUS
CN Benzamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[2-[3{trifluoromethyl)phenyl]ethyl}- (9CI) (CA INDEX NAME)

PAGE 2-A

612529-57-4 HCAPLUS Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-N-(3-methylbutyl)- (9CI) (CA INDEX NAME)

612529-50-5 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-u-(phenylmethyl)-,
1,1-dioxide, (GS)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

612529-59-6 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -(phenylmethyl)-, 1,1-dioxide, { α R}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzoic acid, 4-[(l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylpropyl cster (9CI) (CA INDEX NAME)

612529-63-2 HCAPLUS
Benzoic acid, 2-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

612529-64-3 HCAPLUS
Acetic acid, {4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenoxy}-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-60-9 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

612529-61-0 HCAPLUS Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1)phenoxy}- (9CI) (CA INDEX NAME)

612529-62-1 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-65-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(carboymethoxyl)phenyl]methyl ester (9C1) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

612529-67-6 HCAPLUS
Benzoic acid, 4-[2-[[[4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]amino]ethyl]- (GC INDEX NAME)

PAGE 2-A

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-73-4 HCAPLUS
Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

612529-74-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue 612529-68-7 HCAPLUS Acetic acid, [4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenoxy]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

612529-69-8 HCAPLUS Acetic acid, (4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y)]methyl]phenoxy]-, phenylmethyl ester (9CI) (CA INDEX NAME)

612529-70-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-75-6 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-3-nitro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

612529-76-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{4-ethoxyphenyl}methyl}-, 1,1-dioxide (CA INDEX NAME)

RN 612529-77-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-78-9 HCAPLUS
CN Benzeneacetic acid, 4-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-80-3 HCAPLUS CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-(phenylaminojethyl seter (9CI) (CA INDEX NAME)

RN 612529-81-4 HCAPLUS
CN Benzoic acid, 4-[(),1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-y1)methyl)-,
2-(3-methoxyphenyl)tehyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-79-0 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-phenylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612529-02-5 HCAPLUS

Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl
ester (9CI) (CA INDEX NAME)

RN 612529-83-6 MCAPLUS
CN Benzole acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-84-7 RCAPLUS
CN Benzole acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
3-methoxy-2,2-dimethyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

RN 612529-85-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2,2,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-90-5 HCAPLUS
CN Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)-,
(3-methyl-4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612529-91-6 HCAPLUS CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-86-9 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}-,
3-{dimethylamino}-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-87-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, ([3ak, 45,5k,6a5)-5-(benzoyloxy)hexahydro-2-oxo-2H-cyclopenta[b]furan-4-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (3-chloro-4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

Me
612529-93-8 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
6-ethoxy-6-oxohexyl ester (9CI) (CA INDEX NAME)

RN 612529-94-9 HCRPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
2-(3-chlorophenyl)ethyl ester (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-{3-(trifluoromethyl)phenyl}ethyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

RN 612529-97-2 HCAPLUS
CN D-Phenylalanine, N-{{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}methyl}-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-98-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-([4-[[(phenylmethyl)amino]methyl]phenyl]meth L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-95-0 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(3-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)

RN 612529-96-1 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued y1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-99-4 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
(4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-A

CH2

CH2

CH2

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 2-A

612530-01-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)mothyl]-,
[4-(methoxycarbonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612530-03-7 HCAPLUS Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, 2-phenoxypropyl ester (9CI) (CA INDEX NAME)

612530-04-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[4-(trifluoromethyl)phenyl]methyl ester (9C1) (CA INDEX NAME)

PAGE 1-A

(Continued) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 2-A

612530-02-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-cyclohexyl-2-methylpropyl ester (SCI) (CA INDEX NAME)

PAGE 2-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 2-A

612530-05-9 HCAPLUS Benzoic acid, $4-((1,1)-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, [3-(trifluoromethyl)phenyl|methyl ester (9Cl) (CA INDEX NAME)$

PAGE 1-A

PAGE 2-A

CF3

612530-06-0 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1}-,
2-(4-carboxyphenyl)ethy1 ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 2-A

RN 612530-08-2 HCAPLUS

Benzoic acid, 3-[[{4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl[oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

CO2#

RN 612530-09-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(2-methylpropyl)amino|methyl]phenyl]me thyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-10-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[{4-[(2,2-dimethylpropyl)amino|methyl]pheny
l]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-11-7 HCAPLUS

N Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-y1)methyl]-,
1-naphthalenyleethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612530-13-9 HCAPLUS
CN Benzeneacetic acid, 4-[2-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]amino]ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

NO2

RN 612530-17-3 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-((carboxymethyl)anino|-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-18-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612530-16-2 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
(3-nitrophenyl)methyl ester {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl)oxylmethyl]- [9CI] (CA INDEX NAME)

RN 612530-19-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
[(1,1'-biphenyl]-4-ylmethyl ester (SCI) (CA INDEX NAME)

H S O

PAGE 2-A

PAGE 1-A

RN 612530-20-8 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-,
[4-(acetylamino)phenyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-21-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[2-(phenylmethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (2-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

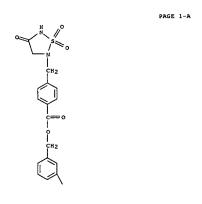
RN 612530-25-3 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl)oxy|methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-22-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[2-methylphenyl]methyl ester (9C1) (CA IMDEX NAME)

RN 612530-23-1 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



PAGE 2-A

CH2-CO2H

RN 612530-26-4 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued) PAGE 1-A

PAGE 2-A

612530-27-5 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)mothyl]-,
(4-fluoro-2-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

RN 612530-28-6 HCAPLUS
CN Benzoic acid,
4-[[5-[12, 4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B

_ OMe

612530-29-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI)
(CA INDEX NAME)

612530-30-0 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(5-methyl-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612530-31-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
2-methylphenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-32-2 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methyl}-,
3-((carboxymethyl)methylamino}-2,2-dimethylpropyl ester (9CI) (CA INDEX
NAME)

RN 612530-33-3 HCAPLUS
Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-,
phenyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-37-7 HCAPLUS
CN 1-Piperazineacetic acid, 4-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9Cl) (CA INDEX NAME)

RN 612530-38-8 KCAPLUS
CN Benzoic acid, 4-(11.-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-,
2-naphthalenyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-34-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, [5-[(2-methyl)propyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-35-5 HCAPLUS
CN Benzole acid, 4-[(],-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenylmethyl ester (9C1) (CA INDEX NAME)

RM 612530-36-6 HCAPLUS CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N,Nbis(2-methylpropyl)- (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-39-9 HCAPLUS
CN 2-Thiophenecarboxylic acid, 5-{[[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}benzoyl]oxy]methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-40-2 HCAPLUS CN Benroic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, [5-(aminocarbonyl)-2-thienyl)methyl ester (9CI) (CA INDEX NAME)

RN 612530-41-3 HCAPLUS
CN Piperazine, 1-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-42-4 HCAPLUS
Benzolc acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(1-oxo-3-yhenylpropyl)-2-thienyllmethyl ester (9C1) (CA INDEX NAME)

612530-43-5 RCAPLUS Bernard 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, [(5-[([phenylmethyl]amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-48-0 MCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-(aminomethyl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-50-4 HCAPLUS
CN Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}(9CI)

(CA INDEX NAME)

612530-51-5 HCAPLUS 1,2,5-Thladiazolidin-3-one, 5-(2,4-dimethoxyphenyl)-, 1,1-dioxide, potassium salt (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-45-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide (9CI) INDEX NAME)

612530-47-9 HCAPLUS Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-52-6P 612530-53-7P 612530-54-8P 612530-55-9P 612530-55-P 612530-55-7 P 612530-65-P 612530-65-P 612530-65-P 612530-66-P 612530-66-P 612530-66-P 612530-66-P 612530-66-P 612530-66-P 612530-66-P 612530-68-4P 612530-69-P 612530-71-9P 612530-72-P 612530-73-1P 612530-73-P 612530-7 612500-7 612530-7 RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (invention compound; preparation of thiazolidinetriones as protein

tyrosine e phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or

mitigate insulin assault and atherosciencis) 612530-52-6 HCAPLUS Acetamide, 2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methylphenoxy]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

612530-53-7 HCAPLUS
1H-1,4-Benzodiszepine-2,5-dione, 3-[[4-(1,1-dioxido-4-oxo-1,2,5-chiadiszolidin-2-y])-3-hydroxyphenyl]methyl]-3,4-dihydro- (9C1) (CA INDEX

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)

RN 612530-54-8 HCAPLUS CN 1,2,5-Thiaddazolidin-3-one, 5-(4-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-55-9 HCAPLUS CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-56-0 HCAPLUS CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)- (9CI) (CA INDEX MAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-60-6 HCAPLUS CN L-Phenylalaninamide, N-benzoyl-O-(dicarboxymethyl)-L-tyrosyl-4-(1,1dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-61-7 HCAPLUS
Senzenepropanamide, α-{{[1,1'-biphenyl]-4-ylsulfonyl)amino}-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued Absolute stereochemistry.

RN 612530-57-1 MCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl)-N-pentyl- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-58-2 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-59-3 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4(carboxymethyl)phenyl]ethyl]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)- (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-62-8 HCAPLUS
CN Benzenepropanamide, a-{{1,1-biphenyl}-4-ylsulfonyl}amino}-4-{1,1-dioxidoid-oxo-1,2,5-chiadiazolidin-2-yl}-N-(4-phenylbutyl)-, (aS}-{9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-63-9 HCAPLUS

Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-Npentyl-a-[(phenylsulfonyl)amino]-, (a5)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

RN 612530-64-0 MCAPLUS
CN Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutl)-u-[(phenylbutlout])-u-[(phenylbutlo

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 612530-65-1 HCAPLUS
CN Benzenepropanamide,
4-(1, 1-dioxido-4-oxo-1, 2, 5-thiadiazolidin-2-yl)-N-(3, 3diphenylpropyl)-a-[(phenylsulfonyl)amino]-, (aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612530-66-2 HCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[(4-aminophenyl]methyl]-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612527-96-5 CMF C9 H11 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

г— c— со₂н

612530-72-0 HCAPLUS 1,2,5-Thiadiazolidin-3-onc, 5-[(1-ethyl-2-methyl-1H-benzimidazol-5-yl]methyl]-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 612528-35-5 CMF C13 H16 N4 O3 S

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-67-3 HCAPLUS
Benzenepropanamide, 3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-N-(4-phenylbutyl)-\alpha-([phenylsulfonyl)amino]-, (\alpha S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 612530-68-4 HCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-69-5 HCAPLUS 1,2,5-Thiadizaclidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-71-9 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-73-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-[(2)-(3-oxo-2(3H)-benzofuranylidene)methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

612530-74-2 HCAPLUS Ethanedione, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl)phenyl- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-75-3 HCAPLUS
9,10-Anthracendione, 2-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y)|methyl|- (9CI) (CA INDEX NAME)

612530-77-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide, sodium salt (9CI)

INDEX NAME)

612530-78-6 HCAPLUS

612530-78-6 HEAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide, trifluoroacetate (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 1

CRN 612530-45-7 CMF C8 H10 N4 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612534-93-7 HCAPLUS L-Phenylalanyl-3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Ed Entered STN: 31 Jul 2002

ACCESSION NUMBER: 2002:555367 HCAPLUS
DOCUMENT NUMBER: 5137:232603

ETITLE: 51ficient Solid-Phase Synthesis of Sulfahydantoins Tremblay, Melanie; Voyer, Normand; Boujabi, Sihem; Dewynter, Georges F.

Control de Rocherche sur la Fonction, la Structure et l'Ingenierie des Proteines, Departement de Chimie, Faculte des Sciences et de Genie, Universite Laval, Quebec, OC, GIK 7P4, Can.

SOURCE: 429-435

CODEN: JCCHFF; ISSN: 1520-4766
American Chemical Society
JOURNET TYPE: JOURNET J

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB A novel solid-phase strategy allows the efficient preparation of traceless sulfahydantoins. A total of 28 derivs., with crude purity generally higher than 85%, were prepared by parallel synthesis. Through reductive alkylations, Mitsunobu reactions, and sulfamoylation reactions on oxime resin, the synthetic strategy affords sulfahydantoin derivs. selectively substituted at N2, e.g., I, N5, e.g., II, and N2, N5, e.g., III, positions, although yields of disubstituted compds. are lower. The mild reaction conditions involved, lead to sulfahydantoins without racemization.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
459831-33-5P 459831-34-6P 459831-35-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of N2,N5-disubstituted sulfahydantoins

reductive alkylation of resin-bound phenylalanine with substituted benzaldehydes and subsequent sulfamoylation, Mitsunobu reaction, resin-cleavage, and cyclization) 459811-31-5 KCAPUUS 1,2,5-Thiediazolidin-3-one, 4-mesthylhenyl]methyl]-4-(phenylmethyl)-2-(2-propenyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-34-6 HCAPLUS
1,2,5-Thladiazolidin-3-one, 2-butyl-5-[(4-methylphenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 459831-35-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{{4-methylphenylmethyl}-4-{phenylmethyl}-2-(3-phenylpropyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

(Continued) ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
283587-14-4P 459831-30-2P 459831-31-3P
459831-32-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of N5-substituted sulfahydantoins via reductive

alkylation of resin-bound phenylalanine with substituted benzaldehydes

and subsequent sulfamoylation, resin-cleavage, and cycliration)

RN 283587-14-4 HCAPLUS

CN 1, 2,5-Thiadiazolidin-3-one,
5-[(4-methoxyphenyl)]methyl]-4-(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-30-2 HCAPLUS
Benzonitrile, 4-{((3S)-1,1-dioxido-4-oxo-3-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

קיים ארביט ארביט

Absolute stereochemistry.

n.yo.r-yc-q mcArUu3 | 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphonyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (4\$)- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Oct 2001
ACCESSION NUMBER: 2001:735235 HCAPLUS
DOCUMENT NUMBER: 136:85785
TITLE: A one-wree court A one-step protocol for the N-chloromethylation of heterocyclic imides Re, Shur Yu, Hongyir Fu, Qinghong: Kuang, Rongze:

AUTHOR(S): Epp,

EPP.

Jeff B.; Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wachita State University, Wichita, KS, 67260, USA

SOURCE: Synthetic Communications (2001), 31(20), 3055-3058

CODEN: SYNCAV; ISSN: 0039-7911

PUBLISHER: Marcel Dekker, Inc.

JOCUMENT TYPE: JOCUMENT TYPE: April 100 CHEM SOURCE(S): CASREACT 136:85785

AB A convenient single step methodol, for the N-chloromethylation of heterocyclic imides using a mixture of formaldehyde sodium bisulfite adduct

heterocyclic imides using a mixture or rormasumine season adduct and thionyl chloride is described. For example, the chloromethylation of 5-Butyl-3-propyl-1, 2,5-thiadiazolidin-3-one 1,1-dioxide gave.

IT 387859-83-8 387859-86-1
RL: RCT (Reactant): RACT (Reactant or reagent)
(preparation of 2-(chloromethyl)-1, 2,5-thiadiazolidin-3-one by chloromethylation of 1, 2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct)

RN 387859-83-8 (RAFBLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 387859-86-1 HCAPLUS CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9P 387859-88-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 300553-85-9 KCAPLUS

30053-85-9 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

387859-88-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 5-(chloromethyl)-4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (9C1) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS

ZZUGOJ-U/-D HANDUN Carbamic acid, {[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester (9CI) (CA

INDEX

RN 220869-16-9 HCAPLUS
CN Carbamic acid,
[2-{[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 13 Jun 2001
ACCESSION NUMBER: 2001:426029 HCAPLUS
DOCUMENT NUMBER: 155:282665
TITLE: Inhibition of serine proteases by functionalized sulfonamides coupled to the

1.2.5-thiadiazolidin-3

sulfonamides coupled to the ne 1,1 dioxide scatfold Groutes, W. C.; He, S.; Kuang, R.; Ruan, S.; Tu, J.; Chan, H.-K. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Bioorganic & Medicinal Chemistry (2001), 9(6), 1543-1548 COODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd. Journal CORPORATE SOURCE:

PUBLISHER: Elsevier Science and DOCUMENT TYPE: Journal English
AB A challenge associated with drug design is the development of selective inhibitors of proteases (serine or cysteine) that exhibit the same primary
substrate specificity, i.e., show a preference for the same Pl residue.
While these proteases have similar active sites, nevertheless there are
subtle differences in their S and S' subsites which can be exploited. We
describe herein for the first time the use of functionalized sulfonamides
as a design and diversity element which, when coupled to the
1.2.5-thiadiazolidin-3-one 1.1 dioxide scaffold yields potent,
time-dependent inhibitors of the serine proteases human leukocyte

cime-dependent inhibitors of the serine proteases human leukocyte elastase

(HLE], proteinase 3 (PR 3) and cathepsin G (Cat G). Our preliminary findings suggest that (a) appending to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold recognition and diversity elements that interact with both the S and S' subsites of a target protease may result in optimal enzyme selectivity and potency and, (b) functionalized sulfonanides constitute a powerful design and diversity element with low intrinsic chemical reactivity and potentially wide applicability. Potent inhibitors of human leukocyte elastase, proteinase 3 and cathepsin G that interact with the S and S' subsites are realized by using functional sulfonamides coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold.

IT 220869-05-6P 220869-07-6P 220869-14-7P 220869-16-9P 365216-43-9P 365216-41-7P 365216-42-9P 365216-43-9P RL: BAC (Biological activity or effector, except adverse); BSU (Biological)

(Biological

ogical study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(Inhibition of serine proteases by functionalized sulfonamides coupled to 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)
220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl]-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA TUNEY NAME)

AMSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM (Continued) 1,2,5-thiadiarolidin-2-yl]methyl](methylsulfonyl)amino]-2-oxoethyl)-, phenylmethyl ester (SCI) (CA INDEX NAME)

RN 365216-39-3 HCAPLUS
CN Benzamide,
N-[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5thiadiazolidin-2-yl]methyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 365216-41-7 HCAPLUS
CN Glycine,
N-[{{4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}(methylsulfonyl)amino]carbonyl]-, ethyl ester
(9CI) (CA INDEX NAME)

365216-42-8 HCAPLUS

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Carbanic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiacolidin-Z-yl]methyl](phenylsulfonyl)-, butyl ester (9CI) (CA
INDEX
NAMEY)

RN 365216-43-9 HCAPLUS
CN L-Phenylalanine, N-[[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-

Absolute stereochemistry.

REFERENCE COUNT:

35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 283587-15-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl)-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-16-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-18-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[4(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS

```
L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN
ED Entered STN: 24 Apr 2001
ACCESSION NUMBER: 135:76831
TITLE:
AUTHOR(S): Albericio, Fernando: Bryman, Lois M.: Garcia, Javier, Michelotti, Enrique L.: Nicolas, Ernesto: Tice, Colin M.

CORPORATE SOURCE: Department of Organic Chemistry, University of Barcelona, Barcelona, 08028, Spain
Journal of Combinatorial Chemistry (2001), 3(3), 290-300
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
Journal of Combinatorial Chemistry (2001), 3(3), 290-300
CODEN: JCCHFF; ISSN: 1520-4766
Afive-step solid-phase synthesis of sulfahydantoins from u-amino acids and aldehydes was developed. The synthetic method allows the use of hindered amino acids, including Val, Phe, and Aib, and use of aromatic aldehydes substituted with electron-withdrawing and -donating groups. Some limitations were encountered with maino acids with reactive side chains. A small but diverse library of compds. was produced for biol. testing.

IT 283587-14-4P 283587-15-5P 283587-16-6P 283587-16-8P 283587-39-0P 346697-33-0P 346697-43-P 346697-51-P 346697-51-P
```

L4 ANSMER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4(1-methylethyl)-,1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-22-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 283587-24-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[2-(methylchio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-35-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(3-chlorophenyl)mechyl}-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-36-7 HCAPLUS Acetamide, N-[4-[{[35}-3-(1-methylethyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-37-8 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 4-(1-methylethyl)-5-{(6-nitro-1,3-benzodioxol-5-yl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) L4

346697-42-5 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[[4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-43-6 HCAPLUS
Acetamide, N-{4-[{(3S}-1,1-dioxido-4-oxo-3-[{4-(phenylmethoxy)phenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-(9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-44-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(6-nitro-1,3-benzodioxol-5-yl]methyl]-4-[[4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346697-38-9 KCAPLUS 1.2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, [45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-39-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[{2-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-40-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

346697-41-4 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2-chlorophenyl)methyl}-4-{{4-(phenylmethoxy)phenyl]methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-45-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-[(4-(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & &$$

RN 346697-46-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{{2,4-dinethoxy-3-methylphenyl}methyl}-4-{{4{phenylmethoxy)phenyl}methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-47-0 HCAPLUS 1,2,3-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[2-(methylthio]ethyl]-, 1,1-dioxide, (4SI- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

346697-48-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl)-4-{2-(methylthio)ethyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-49-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl)-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-50-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[{2-chloro-5-(trifluoromethyl)phenyl]methyl}4-[2-(methylthio)ethyl]-, 1,1-dioxide, (48)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
346697-55-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-56-1 HCAPLUS
1.2,5-Thiadiarolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4[([phenylmethyl]thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-57-2 HCAPLUS
1,2,5-Thiadiracilidine-3-acetic acid, 2-[(3-chlorophenyl)methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-58-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 2-[[4-(acetylamino)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (33)- [9C1] (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-51-6 HCAPLUS
1,2,5-Thiediarolidin-3-one, 5-[(2-chlorophenyl)methyl]-4[((phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (5CI) (CA INDEX NAME)

346697-53-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl)-4[(phenylmethyl)thio]methyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-54-9 HCAPLUS Acctamide, N-(4-[([3R]-1,1-dioxido-4-oxo-3-[([phenylmethyl]thio]methyl]-1,2,5-thiadiazolidin-2-yllmethyl]phenyl)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid,
2-{(4-chloro-3-nitrophenyl)methyl]-4oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-60-7 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[{2,4-dimethoxy-3-methylphenyl|methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, {3S}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-62-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((4-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-63-0 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-({2-(trifluoromethyl)phenyl|methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. .

346697-64-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{l-methylethyl}-5-{{3-}
(trifluoromethyl)phenyl}methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-65-2 HCAPLUS
Benroic acid, 4-[(35)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-73-2 KCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]4-[[4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-74-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl)-4-[(1-(phenylmethyl)-1H-imidazol-4-yl]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-([1-(phenylmethyl)-1H-imidazol-4-yl]methyl]-

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-69-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{3-methylphenyl}methyl]-4-[{4(phenylmethoxy)phenyl}methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-71-0 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 4-[[4-(phenylmethoxy)phenyl]methyl]-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9C1) CCA INDEX

Absolute stereochemistry.

RN 346697-72-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((2,3-dihydro-1,4-benzodioxin-6-y1)methyl]-4-[(4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-76-5 HCAPLUS
CN 1,2,5-Thiadiatolidin-3-one,
5-[(2,3-dihydro-1,4-ben:odioxin-6-y1)methy1]-4[[1-(phenylmethy1)-1H-imidazo1-4-y1]methy1]-, 1,1-dioxide, (45)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

346697-77-6 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-methylphenyl)methyl]-4-oxo-, methyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-79-8 HCAPLUS

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN (Continued)
CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-[{4(trifluoromethyl)penyl)methyl}-, methyl ester, 1,1-dioxide, (35)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 346697-80-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-{(2,3-dihydro-1,4-benzodioxin-6-y1)methyl}-4-oxo-, methyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

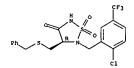
RN 346697-81-2 HCAPLUS
CN Acetamide, N-[4-[{(3S)-3-[2-(methylthio)ethyl]-1,1-dioxido-4-oxo-1,2,5- 'thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-82-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(2-(methylthio)ethyl)-5-((6-nitro-1,3benrodioxol-5-yl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA IMDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued



RN 346697-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(4-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-88-9 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9C1) (CA INDEX
NAME)

Absolute stereochemistry.

4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-83-4 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-[(4-chlorophenyl)methyl)-4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9C1) (CA INDEX NAME)

Sheelute erereechemistry.

$$Ph \qquad S \qquad R \qquad N \qquad O \qquad C1$$

RN 346697-84-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl)-4[((phenylmethyl)thio]methyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-85-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[{2-chloro-5-(trifluoromethyl)phenyl}methyl]4-[{(phenylmethyl)thio]methyl}-, 1,1-dioxide, (4R)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-89-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-{{2-chloro-5{trifluoromethyllphenyl]methyl}-4-oxo-, phenylmethyl ester, 1,1-dioxide,
{3S}- (9CI) CA INDEX NAME}

Absolute stereochemistry.

Absolute stereochemistry.

RN 346697-91-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-{(phenylmethoxy)methyl]-5-{[3-(trifluoromethyl)phenyl]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-92-5 HCAPLUS
Benzoic acid, 4-[([3])-1,1-dioxido-4-oxo-3-[(phenylmethoxy|methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-93-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl]-4-((phenylmethoxy)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-97-0 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346698-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-[[2-(trifluoromethyl)phenyl]methyl], 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346690-04-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-phenyl-5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-05-3 HCAPLUS
Benzoic acid, 4-[((33)-1,1-dioxido-4-oxo-3-phenyl-1,2,5-thiadiazolidin-2-yl]methyll-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1.4 BASWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

346697-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[(3-(trifluoromethyl)phenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-99-2 HCAPLUS
Benzoic acid, 4-{((35)-3-{(4-nitrophenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-00-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl]-4-[(4-nitrophenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346698-06-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-phenyl-1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-12-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{{4-methoxyphenyl}methyl}-4-{{15}-1-methylpropyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-14-4 HCAPLUS
1,2,5-Thiadisrolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4-{[15}-1-methylpropyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 47 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Dec 2000

ACCESSION NUMBER: 2000:898004 HCAPLUS

DOCUMENT NUMBER: 134:307088

114:307088

1,2,5-Thiadiazolidin-3-one 1,1 Dioxide: A Powerful Scaffold for Probing the S' Subsites of (Chymo)trypsin-Like Serine Proteases

Groutas, William C.; Epp, Jeffrey B.; Kuang, Rongze; Ruan, Sumei; Chong, Lee S.; Venkataraman, Radhike;

Tu,

Jun; He, Shu; Yu, Hongy; Fu, Qinghong; Li, Yue He;
Truong, Tien M.; Vu, Nga T.

CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA

SOURCE: Archives of Biochemistry and Biophysics (2001),
385(1), 162-169
CODEN: ABBIA4; ISSN: 0003-9861

PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: Brights
AB The 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) embodies a motif
that allows it to dock to the active site of (chymo)trypsin-like

pases
in a predictable and substrate-like fashion. Consequently, inhibitors
derived from this heterocyclic scaffold interact with both the S and S
subsites of an enzyme. Exploitation of binding interactions with both

Sand S' subsites of a target enzyme may lead to compds. With greatly enhanced enzyme selectivity and inhibitory potency. This preliminary report describes the use of a series of compds. having the heterocyclic scaffold linked to various amino acids to probe the S' subsites of human leukocyte elastase (HLE), proteinase 3 [FR 3], and cathepsin G (Cat G). For comparative purposes, a series of compds. derived from a related scaffold, isothiazolidin-3-one 1,1 dioxide (III), was also generated. Several of the compds. were found to be highly potent and selective time-dependent inhibitors of HLE, FR 3, and Cat G. (c) 2001 Academic Press.

Tress. 334975-68-7P 334975-69-8P 334975-75-6P 334975-81-4P 334975-83-6P 334975-85-8P 334975-88-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical
study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold for probing S'
subsites of human leukocyte elastase, proteinase 3 and cathepsin G)
334975-68-7 HCAPLUS
L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl)-, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

334975-81-4 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl)-, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-83-6 HCAPLUS
L-Phenylalanine, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HC1 334975-85-8 HCAPLUS L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

334975-69-8 HCAPLUS
D-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-, [(45)-4-(2-methylproyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

334975-75-6 HCAPLUS L-Phenylalanine, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 334975-74-5 CMF C23 H29 N3 O5 S

Absolute stereochemistry.

AMSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-1,1-dioxido-3-oxo-4,3-bis(phenylmethyl)-1,2,5-thiadiazclidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-88-1 HCAPLUS D-Phenylalanine, {{45}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]mathyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 334975-87-0 CMF C26 H27 N3 O5 S

Absolute stereochemistry.

2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl-2-oxazolyl)thio]methyl]-4-[2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-[{(5-phenyl-1,3,4-oxadiazol-2-yl]thio|methyl]-, 1,1-dioxide (9CI) (CA INDEX

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 Jul 2000
ACCESSION NUMBER: 2000:488727 HCAPLUS
DOCUMENT NUMBER: 33:277919
Potent inhibition of serine proteases by heterocyclic sulfide defivatives of 1,2,5-thiadiazolidin-3-one 1,1 digital sulfide detivatives of 1,2,5-thiadiazolidin-3-one 1,1
dioxide
AUTHOR(S):

He, S., Kuang, R., Venkstaraman, R.; Tu, J.; Truong,
T. M.; Chan, H. K.; Groutas, W. C.

CORPORATE SOURCE:

Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bisorgamic * Medicinal Chemistry (2000), 8(7),
1713-1717

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER:
DOCUMENT TYPE:
JOURNAL Science Ltd.
JOHNS SOURCE(S):
CASREACT 131:277919

AB The existence of subtle differences in the Sn' subsites of
closely-related
(chymoltrypsin-like serine proteases, and the fact that the
1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold docks to the active site
of (chymoltrypsin-like enzymes in a substrate-like fashion, suggested
that the introduction of recognition elements that can potentially interact with the Sn' subsites of these processes might provide an effective means for optimizing enzyme potency and selectivity. Accordingly, a series of heterocyclic sulfide derivs, based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) was synthesized and the inhibitory activity and selectivity of these compds, toward human leukocyte elastase (HLE), proteinase 3 (PR 3) and cathepsin G (Cat G) were then determined dis. with Pl=isobutyl were found to be potent, time-dependent inhibitors of HLE to a lesser extent PR 3, while those with Pl=benzyl inactivated Cat G rapidly and irreversibly. This study has demonstrated that 1,2,5-thiadiazolidin-3-one 1,1 dioxide-based heterocyclic sulfides are effective inhibitors of (chymolrtypsin-like serine proteases. 220869-26-1P 220869-27-2P 220869-29-4P 220869-30-7P 220869-33-5P 220869-38-5P 220869-38-5P 220869-38-5P 220869-38-5P 220869-38-5P 220869-38-5P 220869-39-6P 220869-40-5P RL: BAC (Biological activity or effector, except adverse); BSU logical and, (Biological

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued) 220869-30-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-26-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4-(2-methylproyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio|methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-35-2 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-2-{{{5-phenyl-2-benzoxzolyl}thio}methyl}-5-{phenylmethyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-39-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-(((5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-40-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-{{{6-amino-2-benzoxazolyl}thio}methyl}-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

of

300553-85-9 RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxide derivative; potent inhibition

serine proteases by heterocyclic sulfide derivs. of thiadiazolidinone dioxide)

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 15 Jun 2000
ACCESSION NUMBER: 2000:395930 HCAPLUS
DOCUMENT NUMBER: 133:159638
TITLE: Utilization of the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold in the design of potent inhibitors

AUTHOR(S):

merine proteases: SAR studies using carboxylates Kuang, R.; Epp. J. B.; Ruan, S.; Chong, L. S.; Venkataraman, R.; Tu, J.; He, S.; Truong, T. M.; Groutas, W. C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (2000), 8(5), 1005-1016
CODEN: BMECEP; ISSN: 0968-0896
Elsevier Science Ltd.
Journal

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

MEMORY TYPE: Journal
UAGE: English
A series of carboxylate deriva. based on the 1,2,5-thiadiazolidin-3-one
1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds has been
synthesized and the inhibitory profile of these compds. toward human
leukocyte elastase (RLE), cathepsin G (Cat G) and proteinase 3 (PR 3) was
then determined Most of the compds. were found to be potent,
-denendent.

then determined Most of the compds. were found to be potent, time-dependent inhibitors of elastase, with some of the compds. exhibiting kinact/KI values as high as 4,928,300 M-l s-l. The inhibitory potency of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform was found to be influenced by both the pKa and the inherent structure of the leaving group. Proper selection of the primary specificity group was found to lead to selective inhibition of HLE over Cat G, however, those compds. that inhibited HLE also inhibited PR 3, albeit less efficiently. The predictable mode of binding of these

compds.

suggests that, among closely-related serine proteases, highly selective inhibitors of a particular serine protease can be fashioned by exploiting subtle differences in their S' subsites.

17 24119-63-1P 281921-30-6P 281921-33-9P 281921-31-39-2P 281921-32-9P 281921-42-0P 281921-45-3P 281921-46-4P 281921-52-2P 281921-45-3P 281921-46-7P 281921-52-2P 281921-54-4P 281921-65-7P 281921-9P RL: BBC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIO1 (Biological study); BIO1 (B

(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis of thiadiazolidinone dioxides and isothiazolidinone dioxides

ides
as serine protease inhibitors)
247179-63-1 RCAPUS
1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-4,5-bis(phenylmethyl)-,
1,1-dioxide, (4\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

REFERENCE COUNT: THIS

THERE ARE 27 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-30-6 HCAPLUS CN Propanoic acid, 2,2-dimethyl-, [4-ethyl-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-33-9 HCAPLUS
Benzeneacetic acid, 4-{[(35)-5-[(2,2-dimethyl-1-oxopropoxy)methyl]-1,1-dioxido-4-oxo-3-propyl-1,2,5-thiadiazolidin-2-yl]methyl]- (9C1) (CA INDEX

NAME)

Absolute stereochemistry.

RN 287921-37-3 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

287921-38-4 HCAPLUS
Benzeneacetic acid, 4-[[(3S)-5-[{2,2-dimethyl-1-oxopropoxy|methyl}-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-39-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-42-0 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 2-[(benzoyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzenepropanoic acid, {(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-54-4 HCAPLUS
Benzeneacetic acid, [{4S}-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 287921-65-7 HCAPLUS
CN Benzoic acid, 2,6-dichloro-,
[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

20/921-91-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-{(acetyloxy)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

287921-45-3 HCAPLUS
Benzoic acid, 2,6-dichloro-,
)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-52-2 HCAPLUS

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

212331-98-1P 212331-99-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxides and isothiazolidinone

(synthesis of man-dioxides
as serine protease inhibitors)
RN 212331-98-1 HCAPLUS
CN 1,25-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylthio)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

212331-99-2 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

FORMAT

THERE ARE 44 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 May 2000
ACCESSION NUMBER: 2000:324184 HCAPLUS
DOCUMENT NUMBER: 133:105000
TITLE: Solid-phase synthesis of sulfahydantoins
Albencio, Pernando: Garcia, Javier; Michelotti,
Enrique L.: Nicolas, Ernestor, Tice, Colin M.
Department of Organic Chemistry, University of
Barcelona, Barcelona, 08028, Spain
Tetrahedron Letters (2000), 41(17), 3161-3163
CODEN: TELEAY; ISSN: 0040-4039
Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

LANGUAGE:

OTHER SOURCE(S):

MENT TYPE: Journal UAGE: English R SOURCE(S): CASREACT 133:105000
A 5-step solid-phase synthesis of 2-unsubstituted 1,2,5-thiadiazolidin-3-one 1,1-dioxides, sulfahydantoins, from Na-Fmoc amino acids and aromatic aldehydes is described. The key step is the base-mediated title

aromatic aldenydes is described. The key step is the base-med; litive cleavage of a resin bound Nd-aminosulfonyl Nd-benzyl amino acid to afford the desired product. This synthesis allows the paration of a diverse library of compds. based on this heterocycle. 283567-14-4P 283587-15-59 283587-16-6P 283587-18-8P 283587-29P 283587-21-3P 283587-22-4P 283587-22-4P 283587-24-F 28358

IT

Absolute stereochemistry.

283587-15-5 HCAPLUS 1,2,5-Thiadizolidin-3-one, 5-[(2,4-dichlorophenyl)methyl)-4-(phenylmethyl)-, 1,1-dioxide, (43)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[{2-chlorophenyl}methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,1,1-dioxide (9CI) (CA IMDEX NAME)

283587-24-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2-chlorophenyl)methyl]-4-{2-(methylthio}ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

14 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

283587-16-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, -methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (48)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-(1-methylethyl)-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

RN 283587-19-9 HCAPLUS CN 1,2,5-fhiadiazolidin-3-one, 5-[{2,3-dihydro-1,4-benzodioxin-6-y1}methy1]-4-(1-methylethy1}-, 1,1-dioxide, {4S}- (9CI) (CA INDEX NAME)

(Continued) L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR 29

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 27 Aug 1999 ACCESSION NUMBER: 1999:536684 HCAPLUS DOCUMENT NUMBER: 131:296963 HUMBER: 151:296963 ACCESSION NUMBER: 1999:536684 RCAPLUS
DOCUMENT NUMBER: 1131:296963
ITITLE: 11296963
AUTHOR(S): Human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold Groutes, William C.; Schechter, Norman M.; Me, Shu; Yu, Hongyi; Huang, Peng; Tu, Juan
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1999), 9(15), 2199-2204
CODEN: BMCLES; ISSN: 0960-894X
DUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of compds. that utilize the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold was synthesized and shown to be highly effective inhibitors of recombinant human skin chymase.

IT 170916-99-7 247178-61-2 247179-63-1
247179-64-2 247179-65-2 247179-66-4
247179-70-0 247179-71-1 247179-72-2
247179-70-0 247179-71-7 247179-72-2
247179-74-2 247179-75-5 247179-76-6
RL: BRC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); PRP (Properties); BIOL (Biological study) (human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)
RN 170918-99-7 RCAPLUS
CN 1,2,5-thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 KCAPLUS
Benzoic acid, 4-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
CN Acetic acid, hydroxy-,
[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 247179-66-4 HCAPLUS
CN Propanoic acid, 2-hydroxy-,
[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiarolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-67-5 HCAPLUS Enterprise Representation (45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiaxolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{acetyloxy}methyl]-4,5-bis(phenylmethyl)-,
1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-64-2 HCAPLUS
Propanedioic acid, mono[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

247179-65-3 HCAPLUS

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

247179-68-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(methylsulfonyl)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-69-7 HCAPLUS
Acetic acid, [[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

247179-70-0 HCAPLUS
Propanoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

247179-71-1 HCAPLUS
Benzoic acid, 2-{[[(43)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-ylmethyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-72-2 HCAPLUS
Benzoic acid, 3-[[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

25

REFERENCE COUNT: THIS

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-74-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-75-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-benzoxazoly1)thio]methyl]-4,5-bis[phenylmethyl]-1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-76-6 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4,5-bis(phenylmethyl)-2-[{(5-phenyl-1,3,4-oxadiazol-2-yl)thio|methyl|-,1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 25 Aug 1999 ACCESSION NUMBER: 1999:529836 HCAPLUS DOCUMENT NUMBER: 131:296959

A General Inhibitor Scaffold for Serine Proteases TITLE:

A General Inhibitor Scaffold for Serine Proteases
a (Chymo)trypsin-Like Fold: Solution-Phase
Construction and Evaluation of the First Series of
Libraries of Mechanism-Based Inhibitors
Kuang, Rongre: Epp, Jeffrey B.; Ruan, Sumei; Yu,
Hongyi: Huang, Peng; He, Shu; Tu, Juan: Schechter,
Norman M.; Turbov, Jane: Froelich, Christopher J.;
Groutes, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Journal of the American Chemical Society (1999),
121(35), 8128-8129
CODEN: JACSAT: ISSN: 0002-7863
American Chemical Society
Journal AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1 dioxide
platform embodies a general motif that renders the platform capable of
binding to the active site of many serine proteases with a
(chymoltrypsin-1ike fold in a predictable fashion and is amenable to the
facile construction of libraries for lead identification and
optimization.
11 170918-99-7P 170919-03-6P 189124-02-5P
247178-39-8P 247178-40-1P 247178-41-2P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (inhibitor; general inhibitor scaffold for serine proteases with a (chymo)trypsin-like fold with solution-phase construction and

(chymo)trypsin-like fold with solution-phase construction and
evaluation
of first series of libraries of mechanism-based inhibitors)
RN 170918-99-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

189124-02-5 HCAPLUS

Absolute stereochemistry.

247178-39-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2(phenylwifonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 16 Mar 1999
ACCESSION NUMBER: 1993:72588 HCAPLUS
DOCUMENT NUMBER: 130:209985
ITITLE: Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as serine protease inhibitors Groutas, William C.; Kuang, Rongze Wichita State University, USA PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: PATENT TYPE: Patent LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE DATE R: DE, GB PRIORITY APPLN. INFO.: A 19970822 US 1997-916693

WO 1998-US17406

w 19980821

OTHER SOURCE(S): MARPAT 130:209985

AB Substituted 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivs. I (R1, R3 = independently H, alkyl, aryl, aralkyl, alkaryl, substituted aryl; R2 = H, alkyl, aralkyl, alkyl, aryl, aralkyl, hydroxyalkyl, amino acid side chain; R4 = H, alkyl, aryl, aralkyl, amino acid side chain; R4 = H, alkyl, aryl, aralkyl, amino acid side chain; R4 = H, alkyl, aryl, aralkyl, aryl, aralkyl, aryl, aralkyl, RCO, COR3, COR1, NHCRATO, NHCOR10, NHCOR10, NHCOR10, NHCHARTO, COR1, Albyl, aryl, aralkyl, KCO, COR3, COO1, NHCHARTO, COR1, NHCHARTO, CONNCHRICORIO, cach q, r = 1-10; Xp = H, G; G = amino protecting group; Y = H, R9, COR9, G; z = 1-10; n = 0-2; K = R9, OR9, NHR9, OCHRYNHY, (NHCHARTO) mOR9, (NHCHARTO) mNR10R17; V = G, H, COCHRYNHY, 2

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247178-40-1 HCAPLUS
1,2,5-Thiadiarolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-5(phenylsulfonyl)methyl]-, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl|methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) = 6, H; m = 1-2; each R7 = amino acid side chain; each R8, R9 = alkyl, aryl, aralkyl, alkaryl, heterocyclyl; each R10-R15 = H, any group R8;

R16, R17 = heterocyclylalkyl; R18 = any group R8, NHR19; R19 = alkyl, aryl, aralkyl; with provisos], oligomers and combinatorial libraries contg. them, and methods of using them, are disclosed. Thus, title

contg, them, and methods of using them, are disclosed. Thus, title id.

If showed apparent second-order rate consts. Kinact/KI (N-1s-1) of 119, 360, 27, 400, and 60 for inhibition of human leukocyte elastase, proteinase 1, and cathepsin G, reap., by in vitro assays.

200869-74-6pp, combinatorial library deriva. 220868-75-Top (combinatorial library deriva. 220868-81-5pp, combinatorial library deriva. 220868-80-4DP, combinatorial library deriva. 220868-81-10p, combinatorial library deriva. 220868-81-5p-2pp (combinatorial library deriva. 220868-89-Topp (combinatorial library deriva. 220868-89-Spp. combinatorial library deriva. 220868-89-20-Pp (combinatorial library deriva. 220868-81-5p-20869-91-7p (combinatorial library deriva. 220869-05-6p (combinatorial library deriva. 220869-05-6p (220869-05-7p 220869-07-9p 220869-07-9p (20869-07-9p 220869-07-9p 220869-07-9p (220869-07-9p 220869-07-9p 220869-07-9p (220869-07-9p 220869-07-9p 220869-07-9p (220869-07-9p (220869-07-9p 220869-07-9p (220869-07-9p (220869-07-9p 220869-07-9p (220869-07-9p (22

RL: BAC (Biological activity or effector, except adverse); BSU

Logical
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid-derived thiadiazolidinone dioxide derivs.

as serine protease inhibitors)
RN 220868-74-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(4-methoxyphenyl)methyl]-,
1,1-dioxide [9CI] (CA INDEX NAME)

CH2C1

220868-75-7 HCAPLUS

kN ZZUB6B-75-/ NCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(3-phenoxyphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-80-4 HCAPLUS
1,2,5-Thiadizolidin-3-one, 2-[(acetyloxy)methyl]-5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220868-81-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(3-phenoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220868-92-8 HCAPLUS
CN L-Phenylalanine,
4-chloro-W-[[[[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-93-9 HCAPLUS
L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl]-

Absolute stereochemistry.

1.4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-86-0 HCAPLUS
Carbamic acid, [[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3-oxo-1,2,5-thiadiarolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX MAME)

220868-87-1 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-5-{[3-phenoxyphenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester [9CI] (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

RN 220868-98-4 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-99-5 HCAPLUS L-Phenylalanine, 4-chloro-N-[[{{1,1-dioxido-3-oxo-5-{{3-phenoxyphenyl}=1,2,5-thiadiazolidin-2-yl|methyl|sulfonyl}methyl}-(GCI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

220869-06-7 HCAPLUS
Carbamic acid, {[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl|methyl](phenylsulfonyl)-, phenylmethyl ester {9CI}(CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220869-19-2 HCAPLUS
CN Glycine,
N-{[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl][phenylsulfonyl)amino]carbonyl)-, ethyl ester
(9CI) (CA INDEX NAME)

220869-20-5 HCAPLUS 220869-20-5 HCAPLOS 1,2,5-Thiadiazolidin-3-one, 2,2'-methylenebis[4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME) ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,]-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](methylaulfonyl)-, butyl ester [9CI] (CA

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-26-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[{(4,5-diphenyl2-2-oxazcly1)thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(5-

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-30-7 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (901) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-{phenylmethyl}-2-[{(3-phenyl-1,2,4-oxadiazol-5-yl)thio}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued) ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-40-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-bentoxazoly1)thio]methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-41-0 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, α -fluoro-3-oxo-4,5-bis(phenylmethy1)-, ethyl ester, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

220869-64-7 220869-65-8
RL: RCT (Reactant), RACT (Reactant or reagent)
(preparation of amino acid-derived thiadiazolidinone dioxide derivs.

serine protease inhibitors)
220869-64-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-2-[{(5-phenyl-2-benzozzolyl)thio]methyl}-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-39-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-{((5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

220869-65-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-61-4P 220869-62-5P 220869-63-6P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derivs.

serine protease inhibitors)

200869-61-4 HCAPLUS

1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dimethylethyl ester, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-62-5 HCAPLUS 1.2.5-Thiadiscolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

1,2,5-Thiadiazolidine-2-acetamide, 4-(2-methylpropyl)-3-oxo-N-(2-phenylethyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

15

REFERENCE COUNT:

THERE ARE 15 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 02 Oct 1998
ACCESSION NUMBER: 1990:622789 HCAPLUS
DOCUMENT NUMBER: 129:289786

TITLE: Kinetics of the hydrolysis of cyclic N-substituted sulfamides: 4-anino-2-cyclohexyl- and 4-anino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5-thiadiazole 11,1-dioxides

AUTHOR(S): Rozas, M. F.; Svartman, E. L.; Mirifico, M. V.; Vasini, E. J.

CORPORATE SOURCE: Instituto de Investigaciones Fisicoquimicas Teóricas

Aplicadas (INIFTA), Facultad de Ciencias Exactas, Departamento de Quimica, Universidad Nacional de La Plata, La Plata, 1900, Argent. Journal of Physical Organic Chemistry (1998), 11(7),

489-494 CODEN: JPOCEE; ISSN: 0894-3230 John Wiley & Sons Ltd. Journal

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

UAGE: English
The hydrolysis reactions of 4-amino-2-phenethyl- and

SOURCE:

slope is observed from pH ca 4 up to the highest exptl. pH (ca 10). The products are the corresponding new compds.: 2-amino-2-(N-substituted-sulfamoyl)isino) acetic acid salts. The C=M bond of these compds. Hydrolyzes further, in a slow reaction, to the sulfamide and oxalic acid derivs. The substrates decompose to the final products without mulation

accumulation
of the acetic acid derivs. under these exptl. conditions. A mechanism is
proposed. Rate consts. and activation parameters are given for the first
reaction step. Owing to steric effects, the reaction rate is higher for
the N-phenethyl-substituted derivative than for the
2-cyclohexyl-substituted
derivative
IT 214216-09-8, 4-Amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5thiadiazole 11.1-dioxide
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
RCT

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006.ACS on STN

ED Entered STN: 05 Aug 1998
ACCESSION NUMBER: 1998:407562 HCAPLUS
1299:216561
Potent and specific inhibition of human leukocyte elastase, cathepsin G and proteinase 3 by sulfone derivatives employing the 1,2,5-thiadiazolidin-3-one 1,1-doxide scaffold
Groutas, William C.; Kuang, Ronger; Ruan, Sumei; Epp, Jeffrey B.; Venkataraman, Radhika; Truong, Tien M. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
SOURCE: Bioorganic & Medicinal Chemistry (1998), 6(6),

SOURCE: 661-671

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd.

PUBLISHER: DOCUMENT TYPE: LANGUAGE: GI Journal English

This paper describes the results of structure-activity relationship studies in a series of heterocyclic mechanism-based inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold (I: Rl * iso-Bu, benzyl; RZ = Bu, Me, benzyl; RZ (RZCOOMEA), etc.; L = SOZPh, SOZCEHRC1-4, etc.) and capable of interacting with the Sn and S'n subsites of a serine proteinase. Sulfone derivs. of I were found to be highly effective, time-dependent inhibitors of human leukocyte elastase (HLE), cathepsin G (Cat C) and proteinase 3 (PR 3). The judicious selection of an Rl group (accommodated at the primary specificity site Sl) that is based on the known substrate specificity of a target serine proteinase, was found to yield highly selective inhibitors. The presence of a benzyl group (R2 = benzyl) at the S2 subsite was found to lead to a pronounced enhancement

inhibitory potency. Furthermore, the effective use of computer graphics and modeling has led to the design of potent, water-soluble inhibitors.

results of these studies demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1-dioxide platform provides an effective means for appending

1,1-dioxide platform provides an effective means for appending recognition
elements in a well-defined vector relationship, and in fashioning highly-selective and potent inhibitors of serine proteinases.

IT 212331-98-19 212331-99-29 212332-00-8P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant) or reagent)
(1,2.5-thiadiazolidin-3-one 1,1-dioxide inhibitors of human leukocyte elastase, cathepsin G and proteinase 3)

RN 212331-98-1 HCAPLUS

ZAZZAJI-YB-1 KCAPLUS 1,2,5-ThiadiazOlidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-(phenylthio)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212332-00-8 HCAPLUS
Benzeneacetic acid, 3-[((3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 212331-79-8P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and
proteinase 3)
RN 212331-79-8 HCAPLUS

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry. Double bond geometry as shown.

170919-03-6 HCAPLUS 1/03/3-03-0 mcArtuo 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-77-6 HCAPLUS
Benzoic acid, 4-[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-78-7 HCAPLUS
Benzoic acid, 4-[{(3S)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5-[(phenylsulfonyl)methyl}-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI) (CA INDEX NAME)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzoic acid, 3-[[(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

170918-99-7P 170919-01-4P 170919-03-6P 212331-77-6P 212331-78-7P 212331-80-1P 212331-81-2P 212331-82-3P 212331-83-4P 212331-66-7P 212331-57-6P 212331-90-3P 212331-92-5P 212331-94-7P 212331-95-8P 212331-97-0P RL: BAC (Biological activity or effector, except adverse); BSU

RL: BAC (Biological activity of extends, energy extends.)

(Biological study, unclassified): SPN (Synthetic preparation): BIOL (Biological study): PREP (Preparation)

(preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3)

RN 170918-99-7 HCAPLUS

CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2
[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-[(28]-3-phenyl-2-propenyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

212331-80-1 HCAPLUS
Benzoic acid, 3-[{(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5((phenylsulfonyl)methyl)-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

212331-81-2 HCAPLUS
Benzoic acid, 2-[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-82-3 RCAPLUS Benzoic acid, 2-(((3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-83-4 HCAPLUS
CN Benzeneacetic acid, 4-{{(3S}-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5-{(phenylsulfonyl)methyl}-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-{[(4-chlorophenyl)sulfonyl]methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- {9CI} (CA INDEX NAME)

Absolute stereochemistry

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-92-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[((3-phenylpropyl)) autionyljmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-94-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[{[3-(tritlucromethyl)phenyl|sulfonyl]methyl}-, 1,1-dioxide, {45}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-95-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-87-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(2-phenylethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[[(4-chlorophenyl]methyl]sulfonyl]methyl]-4{2-methylpropyl)-5-[phenylmethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-97-0 HCAPLUS
CN Benzeneacetic acid, 4-[[(3S]-1,1-dioxido-4-oxo-3-(phenylmethyl)-5[(phenylaulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

```
10510026rtr
L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Apr 1998 ACCESSION NUMBER: 1998:200895 HCAPLUS DOCUMENT NUMBER: 128:278642
                                                                                                                    128:278642
Use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent inhibitors of serine proteinases Kuang, Rongze: Venkataraman, Radhika: Ruan, Sumei: Groutas, William C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1998),
 AUTHOR (S):
 CORPORATE SOURCE:
                                                                                                                      539-544
CODEN: BMCLEB; ISSN: 0960-894X
Elsevier Science Ltd.
Journal
 CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: Brglish

B The attachment of a phosphate leaving group to the

1,2,5-thiadiazolidin-3-
one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds was found
to yield highly potent, time-dependent inhibitors of human leukocyte
elastase (HLE).

IT 205932-85-0P 205932-87-2P 205932-88-3P
205932-89-4P
RL: BBC (Biological activity or effector, except adverse); BSU

(Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
                       logical
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and
isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent
inhibitors of serine proteinases)
205932-65-0 HCAPLUS
Phosphoric acid, dimethyl (4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-
(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX
NAME)
```

Phosphoric acid, dibutyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME) L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 30 Aug 1997 ACCESSION NUMBER: 1997:555602 HCAPLUS 127:257045 127:23:7043 Competitive particle concentration fluorescence immunoassays for measuring antidiabetic drug levels TITLE: in mouse plasma mouse plasma Bright, Stuart W.; Tinsley, Frank C.; Dominianni, Samuel J.; Schmiegel, Klaus K.; Fitch, Lora L.; Gold, AUTHOR(S): Gerald Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA Journal of Immunological Methods (1997), 207(1), CORPORATE SOURCE: 23-31 CODEN: JIMMBG: ISSN: 0022-1759 PUBLISHER: Elsevier DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two competitive particle concentration fluorescence immunoassays were
developed
to measure blood levels of analogs of antidiabetic drugs being tested in
diabetic mics. Ligands that contained the active pharmacophores were
conjugated to PPD for immunization and to F-phycocrythrin for use as
a tracer in the immunoassays. Approx. 90% of 262 compds. assayed were
detectable at less than 120 m in plasma which was well below the therapeutic level of 1 μ M for lowering blood glucose. These data were used to define the bioavailability of test compds. and assist in decisions
of constructing active analogs. Of addnl. interest, we noted
crossreactivity of one monoclonel antibody for 3 different compound that are all known to bind with varying affinities to peroxisome proliferator-activated receptors. 196079-43-3 196079-43-3 RL: ANT (Analyte); ANST (Analytical study) (competitive particle concentration fluorescence immunoassays for

measuring
antidiabetic drug levels in mouse plasma)
RN 196079-43-3 RCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[2-(2-phenyl-4-oxazolyl)ethoxy]phenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME) THERE ARE 13 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: 13 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

205932-88-3 HCAPLUS Phosphoric acid, (4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl bis(phenylmethyl) ester (9CI) (CA INDEX

205932-89-4 RCAPLUS
Phosphoric acid, [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-chiadiazolidin-2-yl]methyl diphenyl ester (9CI) (CA INDEX NAME)

THERE ARE 20 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT:

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Apr 1997 ACCESSION NUMBER: 1997:226843 HCAPLUS DOCUMENT NUMBER: 126:287581 Structure-Based Design of a General Class of McChanism-Based Inhibitors of the Serine Proteinases Employing a Novel Amino Acid-Derived Meterocyclic Scaffold TITLE: AUTHOR(S):

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

DOCUMENT TYPE:

DOCUMENT TYPE:

DOCUMENT TYPE:

DAMAGE TO BE THE SOURCE SEND THE SOURCE SOURCE SOURCE SOURCE.

DOCUMENT TYPE:

DOCUMENT TYPE heterocyclic mechanism-based inhibitors of the serine proteinases that embody in their structure a novel peptidomimetic scaffold (1,2,5-thiadiazolidin-3-one 1,1-dioxide). Sulfone derivs of this class were time-dependent, potent, and highly efficient irreversible inhibitors of human leukocyte elastase, cathepsin G, and proteinase 3. The partition ratios for a select number of inhibitors were found to range between 0 and 1. and 1.
We furthermore demonstrate that these inhibitors exhibit remarkable enzyme
selectivity that is dictated by the nature of the Pl residue and is
consistent with the known substrate specificity reported for these
enzymes. Thus, inhibitors with small hydrophobic side chains were
effective inhibitors of elastase, those with aromatic side chains of
cathepsin G, and those with a basic side chain of bovine trypsin. Taken
together, the findings cited herein reveal the emergence of a general
class of stable mechanism-based inhibitors of the serime proteinases
which which

can be readily synthesized using amino acid precursors. Biochem. and
high-field NMR studies show that the interaction of this class of
inhibitors with a serine proteinase results in the formation of a stable
acyl complex(es) and the release of benzenssulfinate, formaldehyde, and a
low mol. weight heterocycle. The data are consistent with initial
formation
of a Michaelis-Menten complex, acylation of Ser195, and tandem loss of
the

leaving group. The initial RLE-inhibitor complex reacts with water generating formaldehyde and a stable RLE-inhibitor complex. Whether the initial RLE-inhibitor complex also reacts with RLS-inhibitor complex also reacts with RLS-inhibitor complex also reacts with RLS-inhibitor the initial RLE-inhibitor complex also reacts with RLS-inhibitor that this complex is not known at this point. The desirable salient parameters associated with this class of inhibitors, including the expeditious generation of structurally diverse libraries of inhibitors based on I. suggest that this class of mechanism-based inhibitors is of general applicability and can be used in the development of inhibitors of human and viral serine proteinsses of clin. relevance. 170918-99-70 170919-03-6P 189124-00-3P 189124-00-3P RLS BAC (Biological activity or effector, except adverse); BSU logical RI: BAC (Biological activity or effector, except adverse); bas (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and structure activity relations of mechanism-based inhibitors

ANSMER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) of human leukocyte serine proteinases employing a novel amino acid-derived heterocyclic scaffold)
170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylwulfonyl)methyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

189124-00-3 HCAPLUS
1,2,5-Thiadizolidin-3-one, 4-ethyl-5-(phenylmethyl)-2[(phenylmulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylnethyl)-2-([phenylsulfonyl)methyl]-4propyl-, 1,1-dioxide, {4\$}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-04-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{1-methylethyl}-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-06-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-butyl-5-(phenylmethyl)-2-

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 01 Dec 1995
ACCESSION NUMBER: 1995:954574 HCAPLUS
DOCUMENT NUMBER: 123:340140
Novel serine protease inhibitors: derivatives of isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide
INVENTOR(S): Groutas, William C. FATENT ASSIGNEE(S): Wichita State University, USA
POT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: PALDY
ACC. NUM. COUNT: 1

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.									APPLICATION NO.							DATE		
						-												
Wo	WO 9518797					A1 199			50713			WO 1995-US236				19950103		
	W:	AM.	AT.	AU.	BB.	BG.	BR.	BY,	CA.	CH	1. (CN,	CZ,	DE,	DK,	ES,	FI,	GB,
		GE.	HU.	JP.	KE.	KG.	KP.	KR,	ĸz.	LK	. 1	LT.	LU,	LV,	MD,	MG,	MN,	MW,
		NL.	NO.	NZ.	PL.	PT.	RO.	RU,	SD.	SE	:. :	SI.	SK,	TJ,	TT,	UA,	UZ,	VN
	DW.	AT.	BE.	CH.	DE.	DK.	ES.	FR,	GB.	GR		IE.	IT.	LU.	MC,	NL,	PT.	SE
119	5550	139	,	,	Α,	,	1996	0827		US	19	94-	1773	52		1	9940	103
C	2179	913			Al		1995	0713		CA	19	95-2	2179	913		1	9950	103
	9515	000			n .		1005	0801		DII.	10	95.	5001	a .		1	9950	103
										~~		,,,		•		_		
	6863							0205										
	7393									EΡ	19	95-1	9080	03		1	9950	103
EF	7393																	
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	١, :	ΙE,	ΙT,	LI,	LU,	MC,	NL,	PT,
SE																		
JF	0950	9922			т		1997	1007										
AT	2159	38			T		2002	0415		ΑT	19	95-	9080	03		1	9950	103
N2	3297	66			А		2001	0223		NZ	19	98-	3297	66		1	9980	216
PRIORIT																	9940	
										WO	19	95-0	JS23	6		w 1	9950	103

OTHER SOURCE(S): MARPAT 123:340140

Various isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide derivs., e.g. I (X = CR2, (un)substituted NH: Rl = H, alkyl, (un)substituted benzyl, indolylalkyl, etc.; Y = non-steroidal antiinflammatory residue, H, protected amino acid, acyloxy, etc.), and their use to reduce or inhibit the activity of serime proteases, are claimed. The compds. are useful as anti-inflammatory and anti-metastatic agents. For example, 4-benzylisothiazolidin-3-one 1,1-dioxide underwent

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) N-alkylation with CICH25ph and Et3M in MeCN, followed by S-oxidn. with m-ClC6H4C(0)00M in CH2C12 [901], to give title compd. II. In an in vitro assay, II had an apparent 2nd-order inactivation rate const. (kobs/[I]

M-1
s-1) of 960 against cathepsin G. A variety of compds. were prepd. and/or tested against cathepsin G, human leukocyte elastase, and/or proteinase-3.
17 170919-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate: preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-16-1 RCRFUUS
CN 1.2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-(3-phenyl-2-propenyl)-2-(phenylthio)methyl)-, 1,1-dioxide, (5-(E))- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 170919-15-0P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological)
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-15-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4,5-bls(phonylenthyl)-2-[(phonylthio)methyl]-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 170919-03-6 170919-21-8 170919-22-9
RI: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): THU (Therapeutic use): BIOL (Biological study);

USES (Uses)

(Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-03-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-21-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylwifonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

PN 170919-22-9 HCAPLUS

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 153044-45-2P 170918-99-7P 170919-01-4P RL: BAC (Biological activity or effector, except adverse); BSU RE: BAK [Bological activity of effects], except savelers, but (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PRDP (Preparation); USES (Uses) (preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as /s. as serine protease inhibitors)
153044-45-2 MCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170918-99-7 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4,5-bis(phenylmethyl)-2(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-[(2E)-3-phenyl-2-propenyl]-2-((phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:124451 HCAPLUS
DOCUMENT NUMBER: 120:124451
TITLE: Substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides:
a new class of potential mechanism-based inhibitors

οf

human leukocyte elastase and cathepsin G
Groutas, William C.; Kuang, Rongze; Venkataraman,
Radhika
Dep. Chem., Wichita State Univ., Wichita, KS, 67260,
USA
Biochemical and Biophysical Research Communications
(1994), 198(1), 341-9
CODEN: BBRCA9; ISSN: 0006-291X
Journal
English AUTHOR(S): CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: GI

A series of substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides (I, R = benzyl; R1 = H, Me, benzyl, CH2CO2-text-Bu or CH2CO2-benzyl) was prepd, and their in vitro inhibitory activity toward human leukocyte elastase

and

cathepsin G was investigated. These compds. inactivated the 2 enzymes efficiently and in a time-dependent fashion.

IT 153044-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and human leukocyte elastase and cathepsin G inhibition by)
RN 153044-45-2 HCAPLUS
CN 12,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 26 Jan 1991
ACCESSION NUMBER: 1991:23940 HCAPLUS
DOCUMENT NUMBER: 114:23940 HTAPLUS
TITLE: Intra- and intermolecular d-sulf

114:23940
Intra- and intermolecular q-sulfamidoalkylation reactions
Lee, Chai Ho: Kohn, Harold
Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA AUTHOR(S): CORPORATE SOURCE:

USA
Journal of Organic Chemistry (1990), 55(25), 6098-104
CODEN: JOCEAH: ISSN: 0022-3263
Journal
English
CASREACT 114:23940 SOURCE:

DOCUMENT TYPE:

OTHER SOURCE(S):

The utility of α -sulfamidoalkylation processes for the generation of sulfamides has been examined. Both intra- and intermol. α -sulfamidoalkylation transformations were observed to proceed in moderate

Sulfamidoalkylation transformations were observed to proceed in moderate good yields. The generality of these processes has been demonstrated using N.N'-di(sryl-substituted)sulfamides, and the utility of these reactions was examined for the preparation of cyclic sulfamides of novel structure. Thus, reaction of PhCHR/NSCONNIZ with ECOZCCH(OEL)2 in the presence of CF3CO2H gave 744 dichiatetrazocinedicarboxylate tetraoxide I, whereas reaction of 3-MeOCEH4CHZNHSOZNNIZ with ECOZCCH(OEL)2 in CF3CO2H followed by methylation gave benzothadiazepinecarboxylate dioxide II. The crystal structures of I and II were determined 130670-00-7P RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of) 130670-00-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-hydroxy-5-(2-phenylethyl)-, 1,1-dioxide, monosodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

=> log y COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.69	340.84
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-24.75	-24.75

STN INTERNATIONAL LOGOFF AT 14:04:52 ON 21 DEC 2006

Connecting via Winsock to STN

Q2-ALL, L1, L2, Z,Q, R1, R-ALL

Welcome to STN International! Enter x:>

LOGINID: SSPTANAG1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * Welcome to STN International

Web Page URLs for STN Seminar Schedule - N. America NEWS "Ask CAS" for self-help around the clock NEWS 3 AUG 09 INSPEC enhanced with 1898-1968 archive NEWS 4 AUG 28 ADISCTI Reloaded and Enhanced NEWS 5 AUG 30 CA(SM)/CAplus(SM) Austrian patent law changes . NEWS CA/CAplus enhanced with more pre-1907 records 6 SEP 11 NEWS CA/CAplus fields enhanced with simultaneous left and right SEP 21 NEWS truncation CA(SM)/CAplus(SM) display of CA Lexicon enhanced NEWS 8 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates NEWS 9 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine NEWS 10 SEP 25 CEABA-VTB classification code fields reloaded with new SEP 28 NEWS 11 classification scheme OCT 19 LOGOFF HOLD duration extended to 120 minutes NEWS 12 NEWS 13 OCT 19 E-mail format enhanced Option to turn off MARPAT highlighting enhancements available NEWS 14 OCT 23 CAS Registry Number crossover limit increased to 300,000 in NEWS 15 OCT 23 multiple databases The Derwent World Patents Index suite of databases on STN NEWS 16 OCT 23 has been enhanced and reloaded CHEMLIST enhanced with new search and display field NEWS 17 OCT 30 JAPIO enhanced with IPC 8 features and functionality NEWS 18 NOV 03 CA/CAplus F-Term thesaurus enhanced NOV 10 NEWS 19 STN Express with Discover! free maintenance release Version NEWS 20 NOV 10 8.01c now available CAS Registry Number crossover limit increased to 300,000 in NEWS 21 NOV 20 additional databases CA/CAplus to MARPAT accession number crossover limit increased NEWS 22 NOV 20 to 50,000 CAS REGISTRY updated with new ambiguity codes DEC 01 NEWS 23 DEC 11 CAS REGISTRY chemical nomenclature enhanced NEWS 24 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated NEWS 25 GBFULL and FRFULL enhanced with IPC 8 features and DEC 14 NEWS 26 functionality CA/CAplus pre-1967 chemical substance index entries enhanced: NEWS 27 DEC 18 with preparation role CA/CAplus patent kind codes updated DEC 18 NEWS 28 MARPAT to CA/CAplus accession number crossover.limit increased NEWS 29 DEC 18 to 50,000 DEC 18 MEDLINE updated in preparation for 2007 reload NEWS 30

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8 NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 14:02:27 ON 21 DEC 2006

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:03:05 ON 21 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0 DICTIONARY FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10510026RTRexpand.str

```
chain nodes :
7  9  18  19  22  23
ring nodes :
1  2  3  4  5  10  11  12  13  14  15
chain bonds :
1-22  1-23  2-7  4-18  4-19  5-9  9-10
ring bonds :
1-2  1-5  2-3  3-4  4-5  10-11  10-15  11-12  12-13  13-14  14-15
exact/norm bonds :
1-2  1-5  1-22  1-23  2-3  2-7  3-4  4-5  4-18  4-19  5-9
exact bonds :
9-10
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15
```

G1:H,CH3

G2:0,S

G3:0,S,N

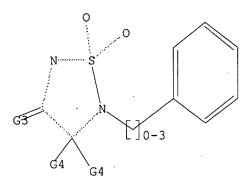
G4:H,CH3 -

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me

G2 0, S

G3 O, S, N

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s 11 SAMPLE SEARCH INITIATED 14:03:30 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 68 TO ITERATE

100.0% PROCESSED 68 ITERATIONS 50 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 866 TO 1854 PROJECTED ANSWERS: 576 TO 1424

L2 50 SEA SSS SAM L1

=> s 11 full FULL SEARCH INITIATED 14:03:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1124 TO ITERATE

100.0% PROCESSED 1124 ITERATIONS 766 ANSWERS

SEARCH TIME: 00.00.01

L3 766 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'HCAPLUS' ENTERED AT 14:03:44 ON 21 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Dec 2006 VOL 145 ISS 26 FILE LAST UPDATED: 20 Dec 2006 (20061220/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 33 L3

=> d ed ibib abs hitstr 1-33

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 03 Aug 2006 ACCESSION NUMBER: 2006:765251 HCAPLUS

DOCUMENT NUMBER: 145:211037

145:211037
Preparation of pyrazolyl aryl ureas as modulators of the protein kinase activation state for treatment of inflammation and hyperproliferative diseases Flynn, Daniel L.; Petillo, Peter A. Deciphera Pharmaceuticals, LLC, USA PCT Int. Appl., 305pp.
CODEN: PIXXD2

INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	PATENT NO.										ICAT		DATE						
WO 2006081034				A2		2006	0803		WO 2	005-		20051223							
WO :	2006	0810	34		A3 200			1123	123										
	w:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE.	EG,	ES,	FI,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS.	JP,	KE.	KG,	KM,	KN,	KP,	KR,		
		KZ,	LC,	LK,	LR.	LS,	LT.	LU,	LV,	LY.	MA.	MD.	MG,	MK,	MN,	MW.	MX.		
		MZ,	NA.	NG.	NI,	NO.	NZ,	OM,	PG,	PH,	PL.	PT.	RO,	RU,	SC,	SD,	SE,		
		SG,	SK.	SL.	SM.	SY,	TJ.	TM.	TN.	TR.	TT.	TZ.	UA,	UG,	US,	UZ,	vc.		
		VN,	YU.	ZA.	ZM.	2W													
	RW:	AT.	BE.	BG.	CH,	CY.	CZ.	DE.	DK.	EE.	ES.	FI.	FR.	GB.	GR,	HU,	IE.		
		IS.	IT.	LT.	LU.	LV.	MC,	NL.	PL.	PT.	RO.	SE.	SI.	SK,	TR.	BF.	BJ.		
							GN,												
							NA.												
		KG.	KZ,	MD.	RU.	TJ.	TM												
TORITY	ADD									115 2	004-	6389	87 P		p 2	0041	223		

MARPAT 145:211037

OTHER SOURCE(S):

Novel compds. and methods of using those compds. for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and

diseases characterized by hypervascularization are provided. In a preferred

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-37-4 HCAPLUS Urea, $N=\{3-(1,1-dimethy|ethy|)-1-\{3-(\{(3R)-3-methy|-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y|]methy|\}phenyl\}-1H-pyrazol-5-yl\}-N'-1-naphthalenyl- (9C1) (CA INDEX NAME)$

Absolute stereochemistry.

872171-57-8 HCAPLUS 2-Naphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA IMDEX MAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) embodiment, the compds. of the invention modulate the activation state of p38 kinase protein, b21 kinase protein, b24 kinase protein, b24 kinase protein, b25 kinase protein. D26 kinase protein. The compds. of the invention I have general formula (R1-(X1))m-A-MH-L-NH-D-(E)q-(Y)t-Q wherein R1 = aryl, heteroaryl, and heterocyclyl; X and Y = individually Q, S, alkynyl, alkenyl, etc.; A = an arom., monocycloheterocyclic, or bicycloheterocyclic ring; D = Ph or a 5-6-membered heterocyclic ring; E = Ph, pyridinyl, or pyrimidinyl; L = -C(O) - or -S(O)2-; j,m,q,t = 0-1; and Q = a substituted ring or ring system. Over 500 compds. were prepd. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester provided the propionate, which was subsequently converted to the hydrazine. Reaction of the hydrazine with 4.4-dimethyl-3-oxopentamenitrile afforded M8

3-(3-tert-butyl-5-amino-IH-pyrisole-1-yl)penyl]propionate, which was coupled with 1-naphthyl isocyanate and reduced to provide urea II. In a competition assay with SKR 86002 as a fluorescent probe, II inhibited p38 MAP kinase with IC50 of

872171-35-2P, 1-[5-tert-Butyl-2-[3-[[(S)-3-methyl-1,1,4-trioxo-IT

{1,2,5}thiadiazolidin-2-yl}methyl}phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-[{(R)-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl}phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-3-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrazol-3-y1]-3-(naphthalen-1-y1)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrazol-3-y1]-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-{1,2,5}thiadiarolidin-2-yl)methyl}phenyl}-2H-pyrazol-3-yl)3-(4-methoxynaphthalen-1-yl)urea
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(p38 kinase inhibitor; preparation of pyrazolyl aryl ureas as

Absolute stereochemistry.

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-62-5 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-{3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl}-1H-pyrazol-5-yl}-N'-1-naphthalenyl-(SCI) (CA INDEX NAME)

872171-63-6 HCAPLUS
Urea, N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-lH-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-39-6 HCAPLUS Urea, N-{3-(1,1-dimethylethyl)-1-[3-[[5-[(4-methoxyphenyl)methyl]-1,1-

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'- (4-fluorophenyl)- (9CI) (CA INDEX NAME)

872171-49-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl}-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-{5-tert-Butyl-2-{3-[{5-(4-methoxybenzyl)-{R})-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2R-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases)
RN 872171-36-3 HCAPLUS
CN Urea. N-[3-(1,1-dimethylethyl)-1-[3-[[(3R)-5-((4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 28 Jul 2006
ACCESSION NUMBER: 2006:739358 HCAPLUS
DOCUMENT NUMBER: 145:377543
TITLE: Isothiazolidinone heterocycles as inhibitors of protein tyrosine phosphatases: Synthesis and structure-activity relationships of a peptide

scaffold AUTHOR(S):

Yue, Eddy W.; Wayland, Brian; Douty, Brent; Crawley, Matthew L.; McLaughlin, Erin; Takvortan, Amy; Wasserman, Zelda; Bower, Michael J.; Wei, Min; Li, Yanlong; Ala, Paul J.; Gonneville, Lucie: Wynn, Richard; Burn, Timothy C.; Liu, Phillip C. C.; Combs, Andrew P. Discovery Chemistry, Experimental Station, Incyte Corporation, Wilmington, DE, 19880, USA Bioorganic & Medicinal Chemistry (2006), 14(17), 5833-5849

CORPORATE SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier B.V.

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: English

SOURCE:

Oxo- and trioxo-substituted isothiazolidinylphenylalanines are prepared

tyrosine mimetics by Suzuki coupling reactions of chloroisothiazolidinones

chloroisothiazolidinones
and chlorodioxoisothiazolidinones with N-Boc-4-borono-L-phenylalanine
derivs.; the isothiazolidinylphenylalanines (with or without subsequent
hydrogenation) are incorporated into dipeptides prepared as human protein
tyrosine phosphatase 18 [PTPIB] inhibitors such as I. of the compds.
tested, I is the most potent inhibitor of PTPIB with an IC50 value of 40
nM; the corresponding mixture of isothiazolidinone diastereomers inhibits
PTPIB with an IC50 value of 80 nM, and the separated

(R)-isothiazolidinone
diastereomer inhibits PTBIB with an IC50 value of 15.5 µM; the related
dipeptides prepared inhibit PTBIB less potently than either I or the
mixture

mixture of isothiazolidine diastereomers containing I. Crystal structures of a

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) dioxochiazolidinone-substituted dipeptide and a dioxocisothiazolinone-substituted dipeptide bound to PTP1B are detd. by X-ray crystallog; the low energy conformation found by ab initio calcns. for the satd. heterocycle more closely approaches the conformation obtained upon inc. L4

heterocycle more closel, -p.,
binding
to PTP1B than that of the unsatd, heterocycle.

IT 850315-22-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(preparation of isothiazolone- and dioxoisothiazolone-substituted
phenylalanine-containing dipeptide amides and their activities as
human

n PTP1B inhibitors) 850315-22-9 HCAPLUS L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl}-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-20-7P 850315-21-8P 850315-23-0P
910606-95-0P 910606-97-2P
REL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of isothiazolone- and dioxoisothiazolone-substituted
phenylalanine-containing dipeptide amides and their activities as

n
PTP1B inhibitors)
850315-20-7 HCAPLUS
850315-20-7 HCAPLUS
Carbamic acid, [(1S)-1-[[4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yliphenylmethyl)-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-21-8 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(3C1) (CA INDEX NAME)

Absolute stereochemistry.

 $850315-23-0 \quad HCAPLUS \\ L-Phenylalaninamide, \quad N-\left[\{4-methoxyphenyl\}acetyl\}-L-phenylalanyl-4-\left[1,1-dioxido-4-xox-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl\}-N-pentyl- (9CI) . (CA INDEX NAME)$

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

910606-95-0 HCAPLUS SIGNOR-YS-U MCAPLUS
Benzenepropanamide, \(\alpha\) amino-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]-N-pentyl-, \((\alpha\))-, mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 910606-94-9 CMF C23 H30 N4 O4 S

Absolute stereochemistry.

2 CM CRN 76-05-1 CMF C2 H F3 O2

(Continued) ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

910606-97-2 HCAPLUS
L-Phenylalaninamide,
senylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl}-N-pentyl-, mono(trifluoroacetate) (9CI) (CA
INDEX NAME)

CRN 910606-96-1 CMF C32 H39 N5 O5 S

Absolute stereochemistry.

2 CM

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT:

THERE ARE 39 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued)

FORMAT

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

AB Title compds. (RIXj)mA(NH)pLn(NH)pDEqYtQ [I; wherein R1 = (un)substituted (hetero)aryl; X, Y = independently O, S, NR6, NR65O2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene, O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h

1-4; A = (un)substituted aryl, hetero(bi)cyclyl; D = (un)substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; E = (un)substituted Ph, pyridinyl, pyrimidinyl; L = CO, SO2;

j, m, n, p, q, t = independently 0, 1; Q = $\{un\}$ substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions]

prepared as p38 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p38 kinase protein comprises the step of contacting the a-C helix, the a-D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation not

not claimed, prepns. and/or characterization data for .apprx.150 examples of

and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester using 10% Pd/C in EtOH provided

propionate, which was treated with NaNO2 in the presence of 6N HCl and SnCl2×2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 3-[3-(3-tert-butyl-5-amino-1H-pyrazole-1-yl)phenyl)propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction

LiOH in THF/MeOH/H2O provided the urea II: In a competition assay with SKF 86002 as a fluorescent probe, the latter inhibited p38 MAP kinase

IC50 of 45 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data). 872171-35-2P, $1-\{5-\text{tert-Butyl-}2-\{3-\{\{\{S\}-3-\text{methyl-}1,1,4-\text{trioxo-}1,1,4-\text$

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-{3-[[(R)-3-methyl-1,1,4-trioxo-{1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-{1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 29 Dec 2005 ACCESSION NUMBER: 2005:1346235 HCAPLUS

144:88279

DOCUMENT NUMBER: Preparation of 1-pyrazolyl-3-phenylurea p38 MAP

INVENTOR(S):

inhibitors as antiinflammatory medicaments Flynn, Daniel L., Petillo, Peter A. USA PATENT ASSIGNEE(S): SOURCE:

U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S. Ser. No. 746,460.
CODEN: USXXCO

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT:

	ENT						DATE				DATE						
US	2005	28821	36		A1 200			0051229 US 20				863	2004070				
US	2004	18090)6		A1		20040916			us 2	003-	20031224					
US	7144	911			B2 200			20040916 US 2003-74 20061205 20060209 WO 2005-US									
WO	2006	0142	90		A2 20060209				1	WO 2	005-	JS23	100		20050630		
WO	2006	0142	90		A3 20060			0427									
	W:										BG,						
											EC,						
											J₽,						
											MG,						
											RO,						
					ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	υz,	vc,	VN,	Υt
			ZM,														
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	F1,	rk,	GB,	GK,	nu,	11
											SE,						
											NE,						
					TJ,			ъь,	54,	12,	00,	ZPI,	۷,	AII,	Α6,	ы,	
ORITY	APP									us :	2003-	7464	60		A2 2	0031	224
										us :	2002-	4373	04P		₽ 2	0021	231
										us :	2002-	4374	0 3 P		P 2	0021	23
										us :	2002-	4374	15P		P 2	0021	23:
										us :	2002-	4374	87 P		P 2	0021	23
										us :	2003-	4638	04P		P 2	0030	41

OTHER SOURCE(S):

MARPAT 144:88279

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl}-2H-pyrazol-3-yl}-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-

3-(4-methoxynaphthalen-1-yl)urea RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIDL (Biological study); PREP (Preparation); USES

(Uses)

(D38 kinase inhibitor; prepn. of (pyrazolyl)(phenyl)urea p38 kinase inhibitors as antiinflammatory agents)
872171-35-2 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-([(3S)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-37-4 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-{3-{{(3R}-3-methyl-1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl]methyl|phenyl|-1H-pyrazol-5-yl}-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-57-8 HCAPLUS

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-Maphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-([1,1-dimixido-4-oxo-1,2,5-thiadimizolidin-2-yl)methyl]phenyl]-lH-pyrazol-5-yl]- (9CI) (CINDEX MAME)

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidid-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9CI) (CA INDEX NAME)

O.21/1-03-0 MCAPLUS
Urea, N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME) 872171-63-6 HCAPLUS

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 872171-36-3P, 1-{5-tert-Butyl-2-[3-[{5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl)-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-[4-fluorophenyl)urea 872171-49-6P, 1-[5-tert-Butyl-2-[3-[[1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant); PREP (Preparation); PREP (Preparation); RACT (Reactant); PREP (Preparation); PREP (Preparation); RACT (Reactant); PREP (Preparation); PREP (Preparation); PREP (Preparation); PREP (Preparation); PREP (Preparation); PREP (Preparation); RACT (Reactant); RACT (Reactant); RACT (Reactant); RACT (Reactant); RACT (Reactant); RACT

Absolute stereochemistry.

872171-39-6 HCAPLUS Urea, N-[3-(1,1-dimethylethyl)-1-[3-[[5-[(4-methoxyphenyl)methyl]-1,1-

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-[1,1-dimethylethyl]-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'- (4-fluorophenyl)- (9CI) (CA INDEX NAME)

872171-49-8 HCAPLUS
Urea, N-[3-[(1,1-dimethylethyl)-1-{3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}phenyl}-1H-pyrazol-5-yl}-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 2-A

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Aug 2005 ACCESSION NUMBER: 2005:904352 HCAPLUS DOCUMENT NUMBER: 143:248386

143:248386
Preparation of substituted azole derivatives for treating diseases mediated by PTPase activity Mjalli, Adnan M. M.; Polisetti, Dharma R.; Subramanian, Govindan; Quada, James C.; Arimilli, Murty N.; Yarragunta, Ravindra R.; Andrews, Robert TITLE: INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

Xie, Rongyuan USA U.S. Pat. Appl. Publ., 204 pp. CODEN: USXXCO Patent English

DOCUMENT TYPE: LANGUAGE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

C.;

	ENT						DATE									ATE	
	2005						2005										
					Al 20050901												
CA	2551	909			A1		2005	0901		CA 2	005-		20050211				
WO	2005	0803	46		A1		2005	0901	,	WO 2	005-1		20050211				
	W:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	Cυ,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NA,	NI,
		NO,	ΝZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ΤJ,	TM,	TN,	TR,	TT,	ΤZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	2W,	AM,
		AZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
					TD,												
EP	1730	118			A1		2006	1213		EP 2	005-	7230	26		2	0050	211
	R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	жU,	IE,
		IS,	IT,	LI,	LT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	AL,	BA,
		HR,	LV,	MK,	YU												
ORITY	APP	LN.	INFO	. :						US 2	004-	5439	71P		P 2	0040	212

WO 2005-US4590 w 20050211

OTHER SOURCE(S):

MARPAT 143:248386

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

The title compds. I [a, b = 0-2; W = 0, S, NR2] (wherein R2 = alkyl,

AB The title compds. I [a, b = 0-2; W = 0, S, NR2 (wherein R2 = alkyl, etc.);

R1 = H, halo, CN, etc.; L1 = a direct bond, (un)substituted NNCO, NNSO2, etc.; Ar1 = (un)substituted (hetero)aryl, fused cycloalkylaryl, etc.; Ar2 = (un)substituted (hetero)arylene, used arylcycloalkylene, etc.; L2 = CH2, O, alkylene, etc.] which can be useful as inhibitors of protein tyrosine phosphatases and thus can be useful for the management, treatment, control, or the adjunct treatment of diseases mediated by PTPase activity such as type I diabetes and type II diabetes, were prepared

Thus, treating

4-(2,4-dichlorophenyl)-2-(2-(4-methoxyphenyl)-(E)-vinyl)-1H-inidazole with Me bromoacetate followed by ester hydrolysis afforded 56% (4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1H-inidazol-iyllacetic acid. The representative compds. I may inhibit PTP-1B with ICSO of less than 20 µM. The pharmaceutical compns. comprising the compds. I, and their use in treating human or animal disorders are also disclosed.

IT 863243-91-8P 863245-57-2P 863245-74-3P 863246-05-3P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation) of substituted arole derivs. for treating diseases mediated by PTPase activity)

RN 86323-91-8 HCAPLUS

CN 1,2,5-ThiadiaZolidin-3-one, 5-(4-[4-(2,4-dichlorophenyl)-2-(1E)-2-[3'-(trifluoromethyl],1,1'-biphenyl]-4-yllethenyl]-1H-imidazol-1-yllmethyl]phenyl-4,4-dimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-57-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyi])-2-[(1E)-2-[3'-(trifluoromethoxy|[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxida (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Double bond geometry as shown.

863245-74-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidarol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\begin{array}{lll} 863246-05-3 & HCAPLUS \\ Benzoic acid, & -[\{4-\{2,4-dichlorophenyl\}-2-\{\{1E\}-2-\{4-\{1,1-dioxido-4-oxo-1,2,5-thidiazolidion-2-y1\}phenyl\}ethenyl]-1H-imidazol-1-y1]methyl]-, \\ methyl ester & (9CI) & (CA INDEX NAME) \\ \end{array}$

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

C

863243-80-5P 863243-92-9P 863243-93-0P
863244-06-6P 863243-95-2P 863244-05-7P
863244-01-1P 863243-95-2P 863244-05-7P
863244-51-7P 863244-47-7P 863244-51-3P
863244-52-4P 863244-53-5P 863245-52-4P
863245-56-1P 863245-56-1P 863245-59-4P
863245-60-7P 863245-61-8P 863245-62-9P
863245-63-0P 863245-61-8P 863245-62-9P
863245-70-9P 863245-61-1P 863245-62-8P
863245-70-9P 863245-71-0P 863245-69-6P
863245-70-9P 863245-71-0P 863245-72-1P
863245-72-3P 863245-71-0P 863245-72-1P
863245-73-4P 863245-71-0P 863245-01-9P
863246-01-0P 863246-01-5P 863246-01-9P
863246-01-0P 863246-11-1P 863246-11-6-6P
863246-10-0P 863246-11-1P 863246-11-6-6P
863287-03-0P
RL: PAC (Pharmacological activity); SPN
(Thermatical Page 1)

B6528/-U3-UP
REL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(preparation of substituted azole derivs. for treating diseases mediated by PTPase activity)

RN 863243-80-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

PAGE 2-A

PAGE 1-A

863243-94-1 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[4-[(4-(2-chlorophenyl)-2-[(1E)-2-(3'-(trifluoromethyl)|1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-92-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-2,4,4-trimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863243-93-0 HCAPLUS 1,2,5-Thiaddazolidin-3-one, 5-[4-[{4-phenyl-2-{(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863243-95-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(4-chloropheny1)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-bipheny1]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-05-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-06-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)]1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-07-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (methylsulfonyl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazol-1-yl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-47-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(3-(rifluoromethyl)phenyl]methyl]-lH-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-51-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-(2-[4-(trifluoromethyl)phenyl]-H-imidazol-1-yl]methyl]phenyl]-,

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

RN 863244-08-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2-chloro-4-fluorophenyl)-2-[(1E)-2[3'-(trifluoromethyl)](1,1'-biphenyl)-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863244-13-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[[3'-

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-52-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[[4-[2,4-dichlorophenyi]-2-[2-[2-fluoro-4{trifluoromethyl}phenyl]ethyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 863244-53-5 HCAPLUS '1,2,5-Thiadizaclidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-(2-[3'-(trifluoromethoxy|[1,1'-bipheny1]-4-y1]ethy1]-H-imidazol-1-y1]methy1]pheny1}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-25-4 HCAPLUS
CN Benroic acid,
4-[[4-(2,4-dichlorophenyl)-2-[{|1E}-2-[3'-(1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-56-1 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, $5-\{4-[(2-\{(1E)-2-(3^*-chloro\{1,1^*-biphenyl)-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-4-1,1-dioxide (9CI) (CA INDEX NAME)$

Double bond geometry as shown.

RN 863245-60-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1-

methylethoxy) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-61-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4'-[(1-exhyl-bchyl)thio][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-Thiadiazolidin-3-one, 5-[4-[(2-[(1E);2-[3',5'-bis[ttrifluoromethyl]fl,1'-bis[henyl]-4-yl]ethenyl]-4-(2,4-dichlorophenyl)lH-imidazol-1-yl]methyl]phenyl}-4, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-58-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(2'-fluoro-5'-propoxy[1,1'-biphenyl]-4-yl]ethenyl}-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

863245-59-4 HCAPLUS

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN y1]methy1]pheny1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-62-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichloropheny1)-2-{(1E)-2-[4'-(1,1-dimethylethyl){1,1'-bipheny1}-4-y1]etheny1}-1H-inidazol-1-y1]methy1]pheny1]- 1,1-dioxide (9CI) (CA INDEX NAME)

bond geometry as shown.

863245-63-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'[1,1-dimethylethyl)-5'-methyl[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-64-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-{[2-{[1E}-2-[4-(5-chloro-2-thienyl)phenyl]-4-(2,4-dichlorophenyl)-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-66-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-([2-[(1E)-2-[4-(5-acetyl-2-thienyl)phenyl])-th-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-69-6 HCAPLUS
(N 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(4,4,4-trifluorobucoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-70-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

RN 863245-68-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-{(1E)-2-[3'-(3,3-dimethylbutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

14 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Con

RN 863245-71-0 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]methyl]-1H-imidazol-2-y1]ethenyl]-4-fluoro[1,1'-biphenyl]-3-y1]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-72-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]2-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-78-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[4(4,4,4-trifluorobutoxy)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(trifluoromethyl)phenoxy]phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-03-1 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(methylsulfony1)[1,1'-bipheny1]-4-y1]etheny1]-1H-imidazol-1-y1]methy1]pheny1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-04-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(1E)-2-[4-(2,4-dichlorophenyl)-1-ethyl1H-inidazol-2-yl]ethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-80-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-{[4-(2,4-dichlorophenyl)-2-{(1E}-2-[4-[4-

(1,1-dimethylethyl)phenoxy]phenyl]ethenyl]-lH-imidazol-1-yl}methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-82-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-{{4-(2,4-dichloropheny1)-2-{{1E}-2-{4-{4-

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 863246-06-4 HCAPLUS
CN Benzoic acid, 4-[[4-(2,4-dichlorophenyl)-2-[[1E]-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-09-7 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)phenyl]methyl]-1H-imidarol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-10-0 HCAPLUS
CArbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1-2,5-thiadiarolidin-Z-yl]phenyl]=nthyl]=1H-imidazol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Double bond geometry as shown.

RN 863246-13-3 HCAPLUS.
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-phenoxyphenyl)-thenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

Double bond geometry as shown.

RN 863246-15-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-

(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-2methylphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863246-11-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(1-

methylethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-12-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichloropheny1)-2-[(1E)-2-(3'-methyl[1,1'-b]heny1]-4-yl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 863246-16-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)][1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-4-propyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863287-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,6-dichlorophenyl)-2-((1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-IH-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 863247-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
mediated by
PTPase activity)
RN 863247-41-0 HCAPLUS
SON Benzoic acid,
4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-, methyl ester (SCI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-89-9 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

692764-94-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

852835-44-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methylphenyl)-, 1,1-dioxide (9CI) (CA

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 May 2005
ACCESSION NUMBER: 2005:378875 HCAPLUS
DOCUMENT NUMBER: 143:19267
TITLE: Structure-based design of protein tyrosine phosphatase-1B inhibitors
AUTHOR(S): Black, Emmar Breed, Jason; Breeze, Alexander L.; Embrey, Kevin; Garcia, Robert; Gero, Thomas W.; Godfrey, Linda; Kenny, Peter W.; Morley, Andrew D.; Minshull, Claire A.; Pannifer, Andrew D.; Reed, Jon; Rees, Amanda; Russell, Daniel J.; Toader, Dorin; Tucker, Julie

CORPORATE SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(10), 2503-2507
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Disevier D.
DOCUMENT TYPE: Journal
LANGUAGE: CASRACCT 143:19267
AB Using structure-based design, a new class of inhibitors of protein tyrosine phosphatase-1B (PTPIB) has been identified, which incorporate the

1, 2, 5-thiadiazolidin-3-one-1, 1-dioxide template.

1,2,5-thiadiazolidin-3-one-1,1-dioxide template. 692765-80-3P

692765-80-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (atructure-based design of protein tyrosine phosphatase-1B inhibitors) 692765-80-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-44-6P 692764-89-9P 692764-94-6P
852835-44-0P 852835-45-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(structure-based design of protein tyrosine phosphatase-1B inhibitors)
612530-44-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852835-45-1 HCAPLUS

107. mentabus 1,2,5-Thiadiazolidin-3-one, 5-(2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA IMDEX NAME)

FORMAT

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2005
ACCESSION NUMBER: 2005:347030 HCAPLUS
DOCUMENT NUMBER: 142:411350

INVENTOR(S): Combs, Andrew P.; Yue, Eddy Wai Tsun; Bower, Michael Jason; Zhu, Wenyu; Crawley, Matchew Lantz; Sparks, Richard Bruce; Pruitt, James Russell; Takvorian, Amy Inc. May Combs, Andrew P.; Tue, Eddy Wai Tsun; Bower, Michael Jason; Zhu, Wenyu; Crawley, Matchew Lantz; Sparks, Richard Bruce; Pruitt, James Russell; Takvorian, Amy Inc. May Composition, USA
DOCUMENT TYPE: Patent Language: Patent Language: English
FAMILY ACC MUM. COUNT: 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

						KIND DATE				APPL								
		2005																
	WO	2005	0355	51		A3		2006	0908									
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN.	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ĖS,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JΡ,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	ΜX,	MZ,	NA,	NI,
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	5G,	SK,	SL,	SΥ,
			ŢJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	vc,	VN,	YU,	ZA,	ZM,	ZW
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
			AZ,	BY,	KG,	KZ,	MD,	RU,	ΤJ,	TM,	AT,	ВĒ,	BG,	CH,	CY,	CZ,	DE,	DK,
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
			SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
				TD,														
	U\$	2005	2727	78		A1		2005	1208		US 2	004-	9603	44		2	0041	007
	US	7141	596			В2		2006	1128									
PRI	ORIT	Y APP	LN.	INFO	.:						US 2	003-	5100	02 P		P 2	0031	800
											US 2	003-	5293	72 P		₽ 2	0031	211
											US 2	004-	6005	06P		₽ 2	0040	811

CASREACT 142:411350; MARPAT 142:411350 OTHER SOURCE(S):

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention provides 1-oxo and 1,1-dioxoisothiazolones (shown

I-TV: also isothiazolidinone analogs of I-TV with R16 and R17 in place of R15 and R2 as a substituent at the 5 position of the isothiazolidinone ring; veriables defined below.e.g. V) and related compds. that can modulate (no data) the activity of a target protein, such as a phosphatase, that selectively binds phosphorylated peptides or proteins. The present compds. can be useful (no data) in treating diseases or

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-(5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]biphenyl-4-sulfonamide 850315-65-58-58-5850315-60-1P, 4-Bromo-H-([13)-2-(14-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-(5-(trifluoromethyl)-1-H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-44-5P, N-{[(18)-2-(4-(1,1-Dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 850315-69-9P, N-{[(18)-2-(4-(1,1-Dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-63-6P, N-{(15)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]biphenyl-4-sulfonamide trifluoroacetate 850315-69-4P

4-Bromo-N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-73-0P, N-[(1S)-2-[3-Chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 850327-65-0P 850327-67-2P, N-[(1S)-1-(5-Chloro-1H-

benzimidazol-2-yl)-2-[3-chloro-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl)-2-cyanobenzenesulfonamide trifluoroacetate 850327-69-4P, N-[(15)-1-(5-chloro-lH-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl)-4-cyanobenzenesulfonamide trifluoroacetate 850327-71-8P,

N-[{1S}-1-{5-chloro-1H-benzimidazo1-2-yl}-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl}pheny]ethyl]-3-phenoxybenzenesulfonamidetrifluoroacetate 690327-73-0P, N-[{1S}-1-{5-chloro-1H-1}]

benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-75-2P, N-[(15)-1-(3-chloro-1H-benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl))-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-77-4P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]-2-(yanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]-4-(yanobenzenesulfonamide trifluoroacetate 805037-83-2P, N-[(1S)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]-4-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]-4-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl]-4-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl-4-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl-4-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thia

2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-85-49,
N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-69, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-89-89,
3-chloro-N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-91-29, N-[(1S)-1-(5-chloro-1H-

benzimidazol-2-y1)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)pheny1]ethy1]-3-fluorobenzenesulfonamide trifluoroacetate

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) disorders, including, for example, diabetes and obesity, that are connected directly or indirectly to the activity of the target protein. Methods of prepn. are claimed and hundreds of example prepns. are included. For example, V was prepd. in 12 steps (50, 62, 100, 59, not detd., 100, 100, 99, not detd., not detd., 43, and 25 % yield) starting from N-tert-butyl-3-[2-(tert-butylcarbamoyl)ethyldisulfanyl]propionamide. For I-IV: a dashed line indicates an optional bond; Scl is a 1st mol. scaffold or is absent; Sc2 is a 2nd mol. scaffold or is absent, wherein

least one of Sc1 and Sc2 is present; or Sc1 and Sc2 together with X1 and X2 or X4 and X5 form a 5-, 6-, or 7-membered fused carbocyclic ring or a 5-, 6-, or 7-membered fused haterocarbocyclic ring; X1 is C or N when Sc1 is present; X1 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc1 is absent; X2 is C or N when Sc2 is present; X2 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N, each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N, each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2 wherein the ring formed by X1, X2, X3, D1, D2, and D3 is an arom. ring; X4 is C or N when Sc1 is present; X4 is O, S, CR3, N, NR4,

CS, SO, or SO2 when Sc1 is absent; X5 is C or N when Sc2 is present; X5

O, S, CR3, N, NR4, CO, CS, SO, or SO2 when Sc2 is absent; X6 is C or N. Each E1 and E2 = O, S, CR3, N, NR4, CO, CS, SO, or SO2, wherein the rin formed by X4, X5, X6, E1, and E2 is an arom: ring; R2 is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl, OR20, SR29, NO2, CN, SOR29, SOR29, COR30, COR031, NR32R331, a 5- or 6-membered heterocarbocyclyl group, or tetrazolyl. R15 is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl,

tetrazolyl: R15 is H, halo, cl-c4 alkyl, C3-c6 cycloalkyl, haloalkyl, OH, C1-C4 alkoxy, C1-C4 haloalkoxy, SH, C1-C4-thioalkoxy, CN, NO2, SO(C1-C4 alkyl), SO(C1-C4 haloalkyl), SO(C3-C6 cycloalkyl), SONR2, SO3H, SO2(C1-C4 alkyl), SO(C1-C4 haloalkyl), SO(C3-C6 cycloalkyl), SONR2, SO3H, SO2(C1-C4 alkyl), CO(C1-C4 alkyl), CO(C1-C4 alkyl), CO(C1-C4 haloalkyl), CO(C1-C4 alkyl), NC(C1-C4 alkyl), CO(C1-C4 alkyl), CO(C1-

phenylpropionyl]amino]-N-pentyl-3-[4-(1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]propionamide 850315-24-[P, N-[(15)-2-[4-(1,1-Dioxido-4-

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Cont. 850327-93-4P, N-[(18)-1-(1H-Benzimidazol-2-y1)-2-[3-chloro-4-dioxido-4-oxo-1, 2, 5-thiadiazolidin-2-y1)phenyl]ethyl]-3-chlorobenzenesulfonamide trifluoroacetate 850327-95-6P, N-[(1S)-1-(1H-Benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-thiadiazolidin-2-y1)phenyl]ethyl]-3-fluorobenzenesulfonamide trifluoroacetate trifluoroacetate RL: PAC (Phermacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; prepn. of 1-oxo and 1,1-dioxoisothiazolone and related modulators of proteins such as phosphatases that bind phosphorylated

peptides and proteins)
850315-19-4 HCAPLUS
L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)-N-pentyl- (9CI) (CA INDEX

Absolute stereochemistry.

850315-22-9 HCAPLUS BB0315-22-9 nCAPLOS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

RN 850315-36-5 HCAPLUS
CN Benzenesulfonamide,
N-((15)-2-(4-(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1)ethyl}-4(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-35-4 CMF C25 H19 F6 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-43-4 CMF C26 H18 F9 N5 O5 S2

Absolute stereochemistry.

RN 850315-48-9 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl]-2{trifluoromethoxy}-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-47-8 CMF C25 H19 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CMF C2 H F3 O2 (Continued)

850315-40-1 HCAPLUS
Benzenesulfonamide, 4-bromo-N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-39-8 CMF C25 H18 Br F6 N5 O6 S2

Absolute stereochemistry.

850315-44-5 HCAPLUS

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 2

76-05-1 C2 H F3 O2

850315-63-6 HCAPLUS [1,1'-Biphenyl]-4-sulfonamide, N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-

1,2,5-thiadiszolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-62-7 CMF C30 H23 C1 F3 N5 O5 S2

Absolute stereochemistry.

r-с-со₂н

850315-65-0 HCAPLUS
Benzenesulfonamide, N-[[1S]-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-4-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (GA INDEX NAME)

CM 1

CRN 850315-64-9 CMF C25 H18 C1 F6 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-73-0 HCAPLUS
Benzenesulfonamide, N-[(1S)-2-[3-chloro-4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-y1)ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-72-9 CMF C26 H17 C1 F9 N5 O5 52

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO2H

RN 850315-69-4 HCAPLUS
CN Benzenesulfonamide,
4-bromo-N-[(15)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl)-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-68-3 CMF C25 H17 Br C1 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 850327-65-0 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1]-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-64-9 CMF C23 H19 C12 N5 O5 S2

RN 850327-67-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-2-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-66-1 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 02

RN 850327-69-4 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-73-0 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-{5-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-72-9 CMF C25 H23 C12 N5 O7 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1]-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-68-3 CMF C24 H18 C12 N6 O5 52

Absolute stereochemistry.

СМ

RN 850327-71-8 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1]-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-70-7 CMF C29 H23 C12 N5 06 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-75-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}ethyl}-3,5-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-74-1 CMF C25 H23 C12 N5 O5 S2

Absolute stereochemistry.

2

со2н

850327-77-4 HCAPLUS

Benzenesulfonamide, N-[(1s)-1-(1H-benzimidazo1-2-y1)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-y1pheny1}ethy1}-,

mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-76-3 CMF C23 H20 C1 N5 O5 S2

Absolute stereochemistry.

ANSWER 6 OF 33 KCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenesulfonamide, N-{(15)-1-(1M-benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido4-4-oxo-1.2,5-thiadiazolidin-2-y1)penyl}ethyl}-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-80-9 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-83-2 HCAPLUS
Benzenesulfonamide, N-[(15)-1-(1H-benzimidazo1-2-y1)-2-{3-chloro-4-(1,1-dioxido-4-cxo-1,2,5-thiadiazolidin-2-y1)pheny1}ethy1}-3-phenoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-82-1 CMF C29 H24 C1 N5 O6 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-79-6 HCAPLUS
Benzenesulfonamide, N-[(15)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-0-xo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-78-5 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-81-0 HCAPLUS

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CRN 76-05-1 CMF C2 H F3 O2

850327-85-4 HCAPLUS
Benzenesulfonamide, N-{(18}-1-(1H-benzimidazol-2-yl)-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-chladiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-84-3 CMF C25 H24 C1 N5 O7 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-87-6 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazo1-2-y1)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3,5-dimethyl-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM ,1

CRN 850327-86-5 CMF C25 H24 C1 N5 O5 S2

Absolute stereochemistry.

СМ 2

CRN ' 76-05-1 CMF C2 H F3 O2

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

 $850327-93-4 \quad HCAPLUS \\ Benzenesulfonamide, N-\{\{1S\}-1-\{1H-benzimidazo1-2-y1\}-2-\{3-chloro-4-\{1,1-dioxido-4-oxo-1,2,5-chladiazolidin-2-y1\}phenyl\}ethyl\}-3-chloro-, mono(trifluoroacetate) {9CI} (CA INDEX NAME)$

CRN 850327-92-3 CMF C23 H19 C12 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

 $850327-89-8\quad HCAPLUS\\ Benzenesulfonamide, 3-chloro-N-{(1S)-1-(5-chloro-lH-benzimidazo1-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-,\\ mono(trifluoroacetate) (9CI) (CA INDEX NAME)$

CRN 850327-88-7 CMF C23 H18 C13 N5 O5 S2

Absolute stereochemistry.

2

RN 850327-91-2 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-1-{5-chloro-1H-benzimidazol-2-y1}-2-{3-chloro-}
4-{1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-y1}phenyl]ethyl]-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-90-1 CMF C23 H18 C12 F N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 76-05-1 CMF C2 H F3 O2

850327-95-6 HCAPLUS
Benzenesulfonamide, N-{(1s)-1-(1H-benzimidazo1-2-y1)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl}ethyl}-3-fluoro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-94-5 CMF C23 H19 C1 F N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 850315-20-7P, [(5)-2-[4-(5-Benzyl-1,1,4-

trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]-1-(pentylcarbamoyl)ethyl]carbamic
acid tert-butyl ester 850315-21-8P, {(1S)-1-{(1S)-2-(4-(5-Benzyl-1,1,4-trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]-1(pentylcarbamoyl)ethyl]carbamoyl)-2-phenylethyl]carbamic acid tert-butyl

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
ester 850315-23-0P, (ZS)-3-[4-(5-Benzyl-1,1,4trioxo[1,2,5]thiadiazolidin-2-yl)phenyl]-2-[[(ZS)-2-[[2-(4methoxyphenyl)acetyl]amino]-3-phenylpropionyl]amino]-N-pentylpropionamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of 1-oxo and 1,1-dioxoisothiazolone and related modulators of
proteins such as phosphatases that bind phosphorylated peptides and
proteins)

proteins such as pnospharases that bind phospholylated peptides amproteins)
850315-20-7 HCAPLUS
Carbamic acid, ((13)-1-[4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]phenyl]methyl)-2-oxo-2-(penylamino)ethyl)-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-21-8 HCAPLUS L-Phenylalaninamide, N-{(1,1-dimethylethoxy)carbonyl}-L-phenylalanyl-4-{1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-23-0 HCAPLUS L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl}-L-phenylalanyl-4-{1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN

ED Entered STN: 11 Apr 2005
ACCESSION NUMBER: 2005:308290 HCAPLUS
DOCUMENT NUMBER: 143:7658
AUTHOR(S): Expedient syntheses of sulfonylhydantoins and two six-membered analogs aix-membered analogs
AUTHOR(S): Campbell, Andrew D. Birch, Alan M. Research and Development, AstraZeneca, Cheshire, SK10 4TG, UK

SOURCE: SYNLES: ISSN: 0936-5214
GOOGN: SYNLES: ISSN: 0936-5214
GOOGN: SYNLES: ISSN: 0936-5214
GOOGN: SYNLES: ISSN: 0936-5214
COENT SYNLES: ISSN: 0936-5214
COEN

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(\$): GI

A range of α -amino esters can be turned into sulfonylhydantoins in a single, atom-economic step using sulfamide and DBU. E.g., reaction of BRHKCH2CO2Et with sulfamide and DBU gave 65% sulfonylhydantoin I. This procedure obviates the need for a three- or four-step sequence utilized AB.

traditional procedures. Two new six-membered analogs [5-aryl-1,2,6-thiadiarinan-3-one 1,1-dioxides and 5-aryl-1,2-thiazinan-3-one 1,1-dioxides], e.g. II and III, have also been prepared utilizing novel synthetic protectols.
612528-23-1P 612529-46-1P 612530-69-5P
852358-50-0P 852358-55-11P 852358-53-3P
852358-54-4P 852358-56-6P 852358-57-7P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (prepn. of sulfonylhydantoins via reaction of amino acid esters with sulfamide and DBU) 612520-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA : INDEX NAME)

612529-46-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2-bromophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

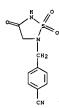
612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA HNDEX NAME)

652358-50-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2-chlorophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-51-1 HCAPLUS 1,2,5-Thladiazolidin-3-one, 5-{(2-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

852358-53-3 HCAPLUS
Benzonitrile, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-(8CI) (CA INDEX NAME)



852358-54-4 HCAPLUS

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: THIS

20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

852358-56-6 HCAPLUS 032330-30-0 ncArbus 1,2,5-Thiadiazolidin-3-one, 5-([1,1'-biphenyl]-3-ylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

852358-57-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-methyl-5-(phenylmethyl)-, 1,1-dioxide, (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 08 Mar 2005
ACCESSION NUMBER: 2005:202894 HCAPLUS
DOCUMENT NUMBER: 142:366767
TITLE: 142:366767
L2,5-7-thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides are potent inhibitors of human

AUTHOR (S):

heterocyclic sulfides are potent inhibitors of hum tryptase
Wong, Tzutshin: Groutas, Christopher S.: Mohan, Swathi: Lai, Zhong: Alliston, Kevin R.: Vu, Nga: Schechter, Norman M.: Groutas, William C. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Archives of Biochemistry and Biophysics (2005), 436(1), 1-7 CODEN: ABBIA4: ISSN: 0003-9861 Elsevier Journal CORPORATE SOURCE:

SOURCE:

PUBLISHER:

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE:

The authors describe herein the design, synthesis, and in vitro biochem.
evaluation of a series of potent, time-dependent inhibitors of the mast
cell-derived serine protease tryptase. The inhibitors were readily
obtained by attaching various heterocyclic thiols, as well as a basic
primary specificity residue Pl, to the 1,2,5-thiadizolidin-3-one
1,1-dioxide scaffold. The inhibitors were found to be devoid of any
inhibitory activity toward a neutral (elastase) or cysteine (papain)
protease, however they were also fairly efficient inhibitors of bovine
trypsin. The differential inhibition observed with trypsin suggests that
enzyme selectivity can be optimized by exploiting differences in the 5'
subsites of the two enzymes. The results described herein demonstrate

versatility of the heterocyclic scaffold in fashioning mechanism-based inhibitors of neutral, basic, and acidic (chymo)trypsin-like serine

IT

proteases. 849415-30-1P 849415-31-2P 849415-32-3P RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

are

potent inhibitors of human tryptase)
849415-30-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-2-[(2-benzoxazolylthio)methyl]-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-31-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-[{(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-32-3 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-[{(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-24-3P 849415-25-4P 849415-26-5P 849415-27-6P 849415-28-7P 849415-29-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

potent inhibitors of human tryptase)
849415-24-3 HCAPIUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

849415-28-7 HCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethy1)-5-[[(5-phenyl-1,3,4-oxadiazol-2-y])thio]methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-29-8 HCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-{phenylmethyl}-5-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

849415-25-4 HCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-26-5 HCAPLUS
Carbamic acid, [4-{(35)-5-{chloromethyl}-1,1-dioxido-4-oxo-2-{phenylmethyl}-1,2,5-thiadiazolidin-3-yl}butyl]-, phenylmethyl ester

(CA INDEX NAME)

Absolute stereochemistry.

RN 849415-27-6 HCAPLUS
CN Carbamic acid,
[4-[(35)-5-[(2-benzoxazolylthio)methyl]-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl)-, phenylmethyl ester
(9CI)

(CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR
THIS

FORMAT

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 19 Aug 2004 ACCESSION NUMBER: 2004:677210 HCAPLUS EN Entered STN: 19 Aug 2004
ACCESSION NUMBER: 2004:677210 HCAPLUS
DOCUMENT NUMBER: 141:235669
TITLE: Potent inhibition of human leukocyte elastase by 1,2,5-thiadiazolidin-3-one 1,1 dioxide-based sulfonamide derivatives
AUTHOR(5): Lai, Zhong; Gan, Xiangdong; Wei, Liuqing; Alliston, Kevin R.; Yu, Hongyir Li, Yue H.; Groutas, William C. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
SOURCE: Archives of Biochemistry and Biophysics (2004), 429(2), 191-197
COODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANOUAGE: CASREACT 141:235669
OTHER SOURCE(5): CASREACT 141:235669
AB The design, synthesis, and in vitro biochem. evaluation of a class of mechanism-based inhibitors of human leukocyte elastase (HLE) that incorporate in their structure a 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold with appropriate recognition and reactivity elements appended to it is described. The synthesized compds. were found to be efficient, time-dependent inhibitors of HLE. The interaction of the inhibitors with HLE is postulated to lead to the formation of a highly reactive N-sulfonyl imine (a Michael acceptor) that arises from an enzyme-induced sulfonamide fragmentation cascade. Subsequent reaction ultimately leads to the formation of a relatively stable acyl enzyme. The results cited herein demonstrate convincingly the superiority of the

1,2,5-thiadiazolidin-3-one
1,1-dioxide scaffold over other scaffolds (e.g., saccharin) in the design of inhibitors of (chymolytrypsin-like serine proteases.

17 749866-31-7P 749966-32-8P 749866-33-9P
749966-31-7P 749966-32-8P 749866-33-9P
749966-31-7P ROPED (Persperties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Properties); Cynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Prepara

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

212331-99-2P 749866-30-6P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (potent inhibition of human leukocyte elastase by

Absolute stereochemistry. Rotation (-).

(potent inhibition of human leukocyte elastase by
1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
RN 212331-99-2 KCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

749866-30-6 HCAPLUS Ethanethiolic acid, S-[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester (9CI) (CA INDEX

Absolute stereochemistry

220869-64-7
RL: RCT (Reactant): RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by
(5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
220869-64-7 HCAPUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-,

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

749866-32-8 HCAPLUS
D-Phenylalanine, N-{[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}sulfonyl}-, methyl ester
(9C1) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-33-9 HCAPLUS
L-Phenylalanine, N-{[[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-34-0 HCAPLUS
L-Phenylalanine, N-[[{(45)-4-{2-methylpropyl})-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl}sulfonyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 30 Jul 2004 ACCESSION NUMBER: 2004:610081 HCAPLUS DOCUMENT NUMBER: 141:157120

141:15/120
Preparation of sulfahydantoins as phosphate isosteres for use as phosphatase inhibitors in the treatment of cancer and autoimmune disorders
Saunders, Jeffrey O.; Miknis, Gregory F.; Blake, TITLE:

INVENTOR(5): James

PATENT ASSIGNEE(S): SOURCE: Vertex Pharmaceuticals Incorporated, USA

PCT Int. Appl., 62 pp. CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

		TENT																
	WO	2004																
		W:										BG,						
			co,	CR,	Cυ,	CZ,	DΕ,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	HU,	ID,	IL.	IN,	IS,	JP,	KÉ,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
			L5.	LT.	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
			PL.	PT.	RO.	RU.	SD.	SE.	SG.	SK.	SL.	TJ,	TM.	TN.	TR,	TT,	TZ,	UA,
								ZA,										
		pw.										52,	TZ.	UG.	ZM.	ZW.	AM.	AZ.
												BG,						
												MC,						
												GQ,						
			ıĸ,	BE,	ы,	Cr,	CG,	CI,	CI1,	un,	G11,	GQ,	J.,	1424,	ruc,	142,	J.,	,
		2511	010			n 1		2004	0778		- 7 2	003-	2511	919		2	0031	230
	LA	2003	010			~1		2004	0010		LA 2	003-	2004	47		2	0031	220
	AU	2003	3004	4/		AI		2004	0010		HU 2	003-	3004	4 /			0031	230
		2004																
	EΡ	1594																
		R:										IT,						
												TR,						
	JР	2006	5149	60		T		2006	0518		JP 2	004-	5666	41		2	0031	230
10	RIT	YAPP	LN.	INFO	.:						US 2	002-	4375	72P		P 2	0021	230
											WO 2	003-	US41	630	1	W 2	0031	230

MARPAT 141:157120

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
4-(1,1,4-Trioxo-[1,2,5]thiadiarolidin-2-yl)benzoic acid methyl ester
729600-47-9P 729600-48-0P 729600-49-1P
729600-50-4P 729600-51-5P 729600-52-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of sulfahydantoins as phosphate isosteres for use as protein

OF

phosphatase inhibitors in treatment of cancer and autoimmune

disorders)

RN 612527-99-8 HCAPLUS

CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

methyl ester (9C1) (CA INDEX NAME)

612530-69-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2

729600-44-6 HCAPLUS Benzoic acid, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl ester (9C1) (CA INDEX NAME)

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ' (Continued)

The invention relates to compds. having a sulfahydantoin or a reverse sulfahydantoin moiety (I) and (II) or pharmaceutically acceptable salts thereof (O = each (un) substituted Cl-8 aliphatic group, C6-10 aryl, heteroaryl having 5-10 ring atoms, heterocyclyl having 3-10 ring atoms; T = Cl-6 alkylidene chain wherein one or two nonadjacent methylene units of T are optionally and independently replaced by O, NR, S, CO, CONR, NRCO, NRCONR, SO, SOZ, NRSOZ, SOZNR, or NRSOZNR: m = 0,1: X = CH2, CO, CF2: R = H or (un)substituted Cl-8 aliphatic group or two R groups bound to the

nitrogen are taken together with the nitrogen to form a 3-7 membered heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen,

heterocyclic ring having 0-z neteroatoms in addition to the mitroyem, ein said heteroatoms are independently selected from N, O, or S}, uses thereof, and related methods. These compds. are inhibitors of phosphatases, particularly inhibitors of protein tyrosine phosphatase SHP-2 and are used in the treatment of various phosphatase mediated diseases such as proliferative diseases, autoimmune disorders, angiogenic disorders, and cancer. The autoimmune disease is selected from glomerulonephritis, rheumatoid archritis, systemic lupus erythematosus, scleroderma, chronic thyroiditis, Graves' disease, autoimmune astritis, diabetes, autoimmune hemolytic anemia, autoimmune neutropenia, thrombocytopenia, atopic dermatitis, chronic active hepatitis, mysthenia gravis, multiple sclerosis, inflammatory bowel disease, ulcerative colitis, Crohn's disease, psoriasis, or graft vs. host disease. The proliferative disease is selected from acute myelogenous leukemia, and

prolificative disease is selected from acute myelogenous leukemia, nic myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple myeloma, and HTLV-1-mediated tumorigenesis. The angiogenic disorder is selected from solid tumors, ocular neovasculization, and infantile haemangiomas. The cancer is selected from colon, breast, stomach, and ovarian cancer. Thus, N-alkylation of Me 4-aminobenzoate by Et bromacateate in the presence of EtN at 60° for 2.5 days gave 4-[[Ethoxycarbonyl]methyl]amino]benzoic acid Me ester which underwent N-sulfamoylation by sulfamoyl chloride in the presence of EtN in CH2C12 at room temperature overnight to give 4-[N-[(Ethoxycarbonyl)methyl]-N-sulfamoylamino]benzoic acid Me ester (III). Cyclization of III by treatment with NaOMe/MeON at room temperature overnight gave 4-[1,1,4-trioxo-1,2,5-thiadiazolidin-2-yl]benzoic acid Me ester (IV). IV showed ICSO of 1.0-100 µM against protein tyrosine phosphatase SHP-2. 612527-99-8P 612530-69-5P 729600-44-6P,

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

729600-47-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

729600-48-0 HCAPLUS
Benzoic acid, 3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,methyl ester (9C1) (CA INDEX NAME)

729600-49-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-phenyl-2-propenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

- CH== CH- Ph

729600-50-4 HCAPLUS Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9c1) (CA INDEX NAME)

NH- (CH2)4-Ph

729600-51-5 HCAPLUS Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

NH-CH2-Ph

729600-52-6 HCAPLUS Benzamide, N-butyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 23 Jul 2004
ACCESSION NUMBER: 2004:589375 HCAPLUS
DOCUMENT NUMBER: 141:140459
ITILE: 1NVENTOR(5): Preparation of sulfamides as anti-cancer agents
INVENTOR(5): Preparation of sulfamides as anti-cancer agents
PATENT ASSIGNEE(5): Deciphera Pharmanaceuticals, Inc., USA
PCT Int. Appl., 160 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE W0 2004060305 A2 20040722 W0 2003-US41425 20031226
W1 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MX, NX, 20, MZ, 0M, PH, PT, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TT, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BM, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, US 2004171075 A1 20040902 US 2003-746545 20031224
US 2004176395 A1 20040909 US 2003-746545 20031224
CA 2511840 A1 20040902 US 2003-746607 20031224
CA 2511840 A1 20040722 CA 2003-2511840 20031226
EP 1590344 A2 20051102 EP 2003-814980 20031226
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NLS, EM, CPT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, RR, BG, CZ, EE, HU, SK
CN 17566849 A 20060405 CN 2003-80110049 20031226
CN 1791596 A 20060621 CN 2003-80110049 20031226
JP 2006519765 T 20060831 JP 2005-508623 20031226
RTYY APPLIN INFO:: US 2002-837304P P 20021231 JP 2006519765 PRIORITY APPLN. INFO.: US 2002-437304P P 20021231 US 2002-437403P P 20021231 US 2002-437415P P 20021231 US 2002-437487P P 20021231 US 2003-463804P P 20030418 US 2003-746545 A 20031224 US 2003-746607 A 20031224 WO 2003-US41425 W 20031226

OTHER SOURCE(S): MARPAT 141:140459 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

$$\bigcap_{Ph} \prod_{Me} \prod_{n=1}^{H} \prod_{n=1}^{O} \prod_$$

Sulfamides, such as I, were prepared for use as anticancer agents which

by modulating the activation states of abl or bcr-abl α -kinase proteins. Thus, 4-MO2CC6H4CH2NNSO2NECOR [R = pyrrolidino], prepared from 4-Meo2CC6H4CH2NH2 and pyrrolidine, was treated with the pyrimidinylaminoantline fragment to give I, which showed 10% inhibition οf

ΙŤ

non-phosphorylated abl kinase at 10µM.
726192-44-5P 726192-45-6P 726192-60-5P
726192-61-6P
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of sulfamides as anti-cancer agents), USES
(preparation of sulfamides as anti-cancer agents), 726192-44-5 RCAPLUS
Benzamide, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-{4-methyl-3-[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl}- (9CI) (CA INDEX NAME)

726192-45-6 HCAPLUS

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-methyl-3-[(4-phenyl-2-pyrimidinyl)amino]phenyl]- (9CI) (CA INDEX NAME)

726192-60-5 HCAPLUS
Benzamide, 4-[(3,3-dimethyl-1,l-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-N-[4-methyl-3-(2-pyrimidinylamino)phenyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612527-99-8P 612528-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfamides as anti-cancer agents)
612527-99-8 HCAPLUS
Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}-,
methy1 ester (9CI) (CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-00-4 HCAPLUS Benzoic acid, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN

ED Entered STN: 18 Jun 2004
ACCESSION NUMBER: 2004:93693 HCAPLUS
141:54348
TITLE: Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as inhibitors of protein tyrosine phosphatase 1B

Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin

Astrazeneca AB, Swed.; Astrazeneca UK Limited
POCUMENT TYPE: CODE: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

English
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATEN	T NO.			KIND DATE					APPL	ICAT		DATE				
			-													
	WO 2004050646															
W	: AE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	ΒY,	ΒZ,	CA,	CH,	CN,
	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ΕG,	ES,	FI,	GB,	GD,	GE,
	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JΡ,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,
	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	ΜX,	ΜZ,	NI,	NO,	ΝZ,
	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ΤJ,	TM,
	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	Yυ,	ZA,	ZM,	ZW		
R	W: BW,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	ΤŹ,	UG,	ZM,	ZW,	AM,	ΑZ,
	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	ÇΥ,	ÇΖ,	DE,	DK,	EE,
	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,
	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	G₩,	ML,	MR,	ΝE,	SN,	TD,
TG																
AU 20	A1		2004	0623												
PRIORITY A	PPLN.	INFO	.:						GB 2	002-	2781	3		A 2	0021	129

WO 2003-GB5120

W 20031126

OTHER SOURCE(S):

MARPAT 141:54348

Title compds. I [wherein Rl = H, (halogeno)alkyl, (hydroxy)alkoxy, alkylamino, etc.; R2 = H, (halogeno)alkyl, halogeno, alkoxy; R3 = alkylamido or (un)substituted alkyl; R4 = H, alkyl, (hetero)aryl; R5 = H

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue Acctamide, N-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methoxyphenyl]methyl)- [9CI) (CA INDEX NAME) (Continued)

705256-61-7 HCAPLUS Butanamide, N-{[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)pheny1]methy1}- (9CI) (CA INDEX NAME)

705256-67-3 HCAPLUS
Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-methyl- (9C1) (CA INDEX NAME)

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) or alkyl; and pharmaceutically acceptable salts thereof) were prepd. as inhibitors of protein tyrosine phosphatase 18 (PTB1B). For example, 5-[4-[acetamidomethyl]-2-methoxyphenyl]-1,2,5-thiadiazolidin-3-one 1,1-dioxide (II) was given in multi-atep synthesis starting from 3-methoxy-4-nitrobenzyl alc. II showed inhibition of human PTB1B with ICSO value of 44µM. Thus, I and their pharmaceutical compns. are useful as inhibitors of protein tyrosine phosphatase 1B for the treatment of diabetes mellitus.

705256-50-4P 705256-54-8P 705256-55-9P
705256-17-1P 705256-67-3P 705256-72-OP
705256-78-6P 705256-82-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

[preparation of 5-phenyl-1,2,5-thiadiazolidin-3-one 1 1-dioxide

{Uses} (Uses) (preparation of 5-phenyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide derivs. as inhibitors of protein tyrosine phosphatase 1B)
RN 705256-50-4 RCAPLUS
CN Acestandie, N-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-54-8 HCAPLUS
Benzeneacetonitrile, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(9CI) (CA INDEX NAME)

705256-55-9 HCAPLUS

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 705256-72-0 HCAPLUS Benzenepentanamide, N-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-78-6 HCAPLUS Acetamide, N-[[4-(3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-82-2 HCAPLUS
Acetamide, N-[2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) alkoxy, C1-6 alkoxy-C1-6 alkoxy, aryloxy, aryl-C1-6 alkoxy, aryloxy-C1-6 alkoxy, heteroaryl-C1-6 alkoxy, c1-6 alkoxy-C1-6 alkoxy-C1-6 alkoxy-C1-6 alkoxy-C1-6 alkylthio-C1-6 alkoxy, C1-6 alkylsulfinyl-C1-6 alkoxy, C1-6 alkylsulfonyl-C1-6 alkoxy, aryl-C1-6 alkylthio, etc.; R2 = H, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, etc.; R2 = H, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, etc.; R2 = H, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, halo; or R1 and R2 together with the carbon atoms to they are attached form a 5-7 membered carbocyclic or heterocyclic ring; and R4 are selected such that (i) R3 = hydrogen, C1-6 alkyl, C1-6 alkyxy, C1-6 alkythio or halo and R4 = aryl, biaryl, heteroaryl, C2-6 alkynyl, c3-7 cycloalkyl, arylcarbonyl, heteroarylarc2-6 alkynyl, arylc-2-6 alkynyl or heteroaryl-C2-6 alkenyl; or (ii) R4 = H, C1-6 alkyl, C1-6 alkynyl, C1-6 alkyl, c1-6 alkyl, c1-6 alkyl, c1-6 alkyl, c2-6 alkynyl, arylc-2-6 alkynyl, arylc-2-6 alkynyl, arylc-2-6 alkynyl, arylc-2-6 alkynyl, arylc-2-6 alkynyl, c2-6 alkynyl, arylc-2-6 alkynyl, c2-6 alkynyl, c3-7 cycloalkyl, arylc-2-6 alkenyl alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6 alkenyl, aryl-c2-6 alkynyl or heteroaryl-c2-6 alkenyl; RS = H, C1-6
alkyl,
C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkyl, halo; R6 = H, C1-6 alkyl;
wherein any aryl, biaryl or heteroaryl group is optionally substituted]
are prepd. These compds. are useful as inhibitors of protein tyrosine
phosphatase PTP1B for the treatment of diabetes mellitus. Thus,
4-tolylboronic acid was coupled with 5-(4-bromophenyl)-1,2,5thiadiazolidin-3-one in the presence of
tetrakis(triphenylphosphine)pallad
ium(0) [Pd(PPh3)4] and cesium carbonate in a mixt. of DMF, DME, EtOH, and
H2O at 170° for 600 s to give 5-(4'-Methyl-1,1'-biphenyl-4-yl)1,2,5-thiadiazolidin-3-one 1,1-dioxide.
17 692765-08-59 692765-17-69
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); RACT (Reactant or reagent); USES (Uses)
(Preparation of phenylthiadiazolidinones as inhibitors of protein
tyrosine

vine
phosphatase lB (PTPIB) for treatment of diabetes mellitus)
692765-08-5 HCAPLUS
[1,1'-Biphenyl]-4-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

HCAPLUS [1,1'-Biphenyl]-3-carboxylic acid, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 21 May 2004 ACCESSION NUMBER: 2004:412929 HCAPLUS DOCUMENT NUMBER: 140:423678 Preparation of 5-(substituted phenyl) thiadiazolidin-3ones as inhibitors of protein tyrosine phosphatase 18 Birch, Alan Martin; Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 89 pp. CODEN: PIXXD2 Patent INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: English LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. KIND DATE A1 20040521 PATENT NO. DATE 2004041799 Al 20040521 W0 2003-GB4721 20031103
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
LR, LS, LT, LU, LV, MA, MD, MG, MK, NN, MM, MX, MZ, NI, NO, NZ,
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BM, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, TI, LU, MC, NL, PT, RO, SE, SI, SK,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, WO 2004041799 AU 2003278392 PRIORITY APPLN. INFO.: Al 20040607 AU 2003-278392 GB 2002-25986 20031103 A 20021107 WO 2003-GB4721 W 20031103 OTHER SOURCE(S):

MARPAT 140:423678

AB The title compds. (I) or pharmaceutically acceptable salts thereof [R1 = H, halo, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkyl, halo-C1-6 alkoxy, halo-C1-6 alkylthio, hydroxy-C1-6 alkoxy, dihydroxy-C1-6 . .

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-76-4P 692764-87-5P 692764-78-6P
692764-78-7P 692764-80-0P 692764-81-1P
692764-82-2P 692764-88-3P 692764-84-4P
692764-81-5P 692764-88-6-6P 692764-87-7P
692764-81-3P 692764-89-9P 692764-90-2P
692764-91-3P 692764-99-0P 692764-93-5P
692764-91-3P 692764-99-0P 692764-93-5P
692764-91-3P 692765-01-8P 692764-99-1P
692765-00-7P 692765-01-8P 692765-02-9P
692765-00-3P 692765-01-4P 692765-02-9P
692765-01-0P 692765-01-4P 692765-02-9P
692765-10-9P 692765-11-0P 692765-02-9P
692765-10-3P 692765-11-0P 692765-12-1P
692765-13-2P 692765-11-0P 692765-12-1P
692765-13-2P 692765-12-1P 692765-12-1P
692765-13-2P 692765-12-1P 692765-12-1P
692765-13-4P 692765-12-1P 692765-13-1P
692765-13-6P 692765-13-1P 692765-13-4P
692765-13-6P 692765-13-1P 692765-13-4P
692765-13-6P 692765-13-6P 692765-14-5P
692765-13-6P 692765-13-6P 692765-14-5P
692765-13-6P 692765-13-6P 692765-14-P
692765-13-6P 692765-14-5P 692765-14-P
692765-13-6P 692765-15-6P 692765-14-P
692765-13-6P 692765-15-6P 692765-16-P
692765-13-6P 692765-15-1P 692765-16-P
692765-13-6P 692765-16-1P 692765-16-P
692765-13-6P 692765-60-9P 692765-61-OP
692765-74-5P 692765-60

phosphatase 1B (PTP1B) for treatment of diabetes mellitus) 692764-76-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

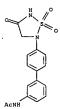
RN 692764-77-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-nitro[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

H O

RN 692764-78-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-dichloro[1,1'-biphenyl]-4-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-81-1 HCAPLUS
CN Acetamide, N-[4'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl){1,1'-biphenyl}-3-yl}- (9CI) (CA INDEX NAME)



RN 692764-82-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-83-3 HCAPLUS
CN 1,2,5-Thiadiazolidiu-3-one, 5-(3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-79-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-80-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

RN 692764-84-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(methylthio)[1,1'-biphenyl]-3-yl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-85-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-86-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-87-7 HCAPLUS
CN Acetamide, N-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl){1,1'-biphenyl}-3-yl}- (9CI) (CA INDEX NAME)

RN 692764-88-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[3-(2-benzofuranyl)phenyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 692764-89-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-93-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-4-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-94-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-95-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-90-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[3-(5-oxazolyl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-91-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-cyclohexylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-92-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-benzoylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

14 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 692764-96-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4,4'-dimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-97-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-4'-phenoxy[1,1'-bipheny1]-3-y1)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692764-98-0 HCAPLUS
CN [1,1'-Biphenyl]-3-carbonitrile,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692764-99-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-nitro[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-00-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-01-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-hydroxy-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-05-2 HCAPLUS
CN Acetamide, N-{3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy{1,1'-biphenyl}-3-yl}- (9CI) (CA INDEX NAME)

RN 692765-06-3 HCAPLUS
CN 1,2,5-Thiadiazolidius-3-one, 5-(4-methoxy-3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-07-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-02-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4,4'-trimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-{trifluoromethyl}[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-04-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[5-(1,3-benzodioxol-5-yl)-2-methoxyphenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-09-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[[1E]-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-10-9 HCAPLUS CN 1,2,5-Thiddiazolidin-3-one, 5-[2-methoxy-5-(2-naphthalenyl)phenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-11-0 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-[4'-(hydroxymethyl)-4-methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Neo CH2-OH

RN 692765-12-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (SCI) (CA INDEX NAME)

Meo CH2-OME

RN 692765-13-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

MeO N O-CHO-Ph

RN 692765-14-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-methoxy-4'-(phenylmethoxy) [1,1'-biphenyl]3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Meo CH2-OMe

RN 692765-19-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methowy-3'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

HeO Neo

RN 692765-20-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy{1,1'-biphenyl}-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO O-CH₂-Ph

RN 692765-15-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(12)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

H O Z Ph

RN 692765-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-[(1,1-dimethylethoxy)methyl]-4methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

Мео — СH2-ОВи-с

RN 692765-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Heo N

RN 692765-22-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-difluoro-4-methoxy[1,1'-biphenyl]-3yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-23-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(5'-fluoro-2',4-dimethoxy{1,1'-biphenyl}-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

H ON

RN 692765-24-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1':3',1''-terphenyl]-3-yl)-,
1,1-dloxide (901) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-25-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-fluoro-4-methoxy{1,1'-biphenyl}-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(1,1-dimethylethyl)-4-methoxy(1,1'-biphenyl)-3-yl|-, 1,1-dioxide (9CI) (CA INDEX NAME)

14 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{5-{(1E)-2-(4-chlorophenyl)ethenyl}-2-methoxyphenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-33-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-ethenyl-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME) 14 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-28-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy(1,1':4',1''-terphenyl)-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-29-0 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 5-(3'-chloro-4'-fluoro-4-methoxy[1,1'-biphenyl]-3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-30-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1':4',1''-terphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-furanyl)-2-methoxyphenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-35-8 HCAPLUS CN 1,2,5-Thiddiazolidin-3-one, 5-(5-benzo[b]thien-2-yl-2-methoxyphenyl)-, 1,1-dioxide (901) (CA INDEX NAME)

RN 692765-36-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-benzofuranyl)-2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-37-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-38-1 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-39-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[1H-pyrazol-4-yl)phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-40-5 HCAPLUS CN Pyrrolidine, 1-[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy(1,1'-5tpheny1)-4-y1)carbony1]- (SCI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-44-9 HCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, N-cyclohexyl-3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-45-0 HCAPLUS
CN 1,2,8-Thisdiazolidin-3-one, 5-(3'-amino-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 692765-46-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4'-(dimethylamino)-4-methoxy[1,1'-biphenyli3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-41-6 HCAPLUS CN [1,1'-Bipheny]1-4-propanoic acid, 3'-{1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-y1)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-42-7 HCAPLUS
CN Carbamic acid, [(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA
INDEX NAMZ)

RN 692765-43-8 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Conti

RN 692765-47-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(4-pyridinyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-48-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-hydroxy-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-49-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(1H-indol-6-yl)-2-methoxyphenyl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-50-7 HCAPLUS
CN 1.2.5-Thladiazolidin-3-one, 5-(2-methoxy-5-(2-thienyl)phenyl)-,
1.1-dioxide (927) (CA INDEX NAME)

RN 692765-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(phenylethynyl)phenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

N 692765-52-9 HCAPLUS
N 1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-(3-phenyl-1-propynyl)phenyl}-,
1,1-dioxide (901) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-56-3 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

RN 692765-57-4 HCAPLUS

Enzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methoxy)-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

RN 692765-58-5 HCAPLUS
CN Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny]]-4-yl]methoxy]-6-hydroxy- (SCI) (CA INDEX NAME)

14 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-53-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-ethynyl-2-methoxyphenyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME) :

RN 692765-54-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methyl[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

RN 692765-55-2 HCAPLUS
CN Benzoic acid, 2-{2-{3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-4'-methoxy{1,1'-biphenyl}-3-yl}ethoxy|-6-hydroxy- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \end{array}$$

RN 692765-59-6 HCAPLUS
CN Benzoic acid, 2-[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'-methoxy[1,1'-biphenyl]-4-yl]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 692765-60-9 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]ethoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

RN 692765-61-0 HCAPLUS
CN Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-4-y1]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-62-1 RCAPLUS
Benzoic acid, 2-(3-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy(1,1'-bipheny1)-3-y1)propoxy1-6-hydroxy- (9C1) (CA INDEX NAME)

692765-63-2 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1}-3-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-64-3 HCAPLUS
Benzoic acid, 2-[3-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-bipheny1]-4-y1]propoxy]-6-hydroxy- (9C1) (CA INDEX NAME)

692765-65-4 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy(1,1'-biphenyl]-4-yl)propoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

(Continued)

692765-66-5 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-bipheny1]-3-y1]methoxy[-6-hydroxy- (9CI) (CA INDEX NAME)

RN 692765-67-6 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin2-yl)-4'-methoxy-N-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-68-7 HCAPLUS
CN Benroic acid,
2-[2-[[[3]"-[4],-[dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]ethoxy[-6-hydroxy-, methyl
ester [9CI] (CA INDEX NAME)

RN 692765-69-8 HCAPLUS
CN Benzoic acid,
C13-[[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]carbony1]amino]propoxy]-6-hydroxy-, methyl
ester (9C1) (CA INDEX NAME)

RN 692765-70-1 HCAPLUS

CN Benzoic acid,
2-[[5-[[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-3-y1]carbonyl]amino]pentyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-71-2 HCAPLUS
CN Benzoic acid,
2-[[6-[[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]carbony1]amino]hexy1]oxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX NAME)

RN 692765-72-3 HCAPLUS

Benzoic acid,
2-[2-[[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-biphenyl]-4-y1]carbonyl]amino]ethoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

RN 692765-73-4 HCAPLUS
CN Benzoic acid,
2-[3-[[[3'-[1],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl]carbonyl]amino]propoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-74-5 HCAPLUS
CN Benzoic acid,
2-[[5-[([3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]carbony1]amino]penty1]oxy]-6-hydroxy-, methy1
ester (9CI) (CA INDEX NAME)

692765-75-6 HCAPLUS

692765-79-0P 692765-80-3P 692765-84-7P 692765-85-8P 692765-86-9P 692766-02-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of phenylthiadiazolidinones as inhibitors of protein

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN methoxyphenyl]- (9C1) (CA INDEX NAME) (Continued)

692765-86-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{2-methoxy-5-{4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

692766-02-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(5-iodo-2-methoxyphenyl)-, 1,1-dioxide (9CI)

(CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phosphatase 18 (PP1B) for treatment of diabetes mellitus)
RN 692765-79-0 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-(4-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-80-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-84-7 RCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-(5-bromo-2-methoxyphenyl)-, 1,1-dioxide (9CT) (CA INDEX NAME)

692765-85-8 HCAPLUS Boronic acid, [3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 10 Oct 2003
ACCESSION NUMBER: 2003:796679 HCAPLUS
DOCUMENT NUMBER: 139:307766
TITLE: Preparation of substituted 1,1-dioxo-1,2,5thiazolidine-3-ones as protein tyrosine phosphatase

and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis Coppola, Gary Mark, Davies, John William; Jewell, Charles Francis, Jr.; Li, Yu-Chin; Wareing, James Richard; Sperbeck, Donald Mark; Stams, Travis Mathew; Topiol, Sidney Wolf, Vlattas, Isidoros Novartis A.-G., Switz.; Novartis Pharma G.m.b.H. PCT Int. Appl., 148 pp. CODEN: PIXXD2 Patent 1b

INVENTOR (S):

PATENT ASSIGNEE(5): SOURCE:

DOCUMENT TYPE: Patent English 1 LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

								APPLICATION NO.									
								WO 2003-EP3466									
											, BG,						
											, EE,						
											, KP,						
											, OM,						
											, US,						
	RW:										, AT,						
		DK.	EE.	ES,	FI,	FR,	GB,	GR,	HU,	1E	, IT,	LU,	MC,	NL,	PT,	RO,	SI
		SI.	SK,	TR													
CA	2480562				A1 20031009			CA 2003-2480562 AU 2003-224030						20030402			
ΑU	2003224030			A1	A1 20031013			AU 2003-224030						20030402			
							US 2003-405728										
ΕP	1492	780			A1		2005	0105		EΡ	2003-	7204	12		2	0030	402
	R:	AT,	BE,	CH,	ÐΕ,	DK,	ES,	FR,	GB,	GR	, ІТ,	LI,	LU,	ΝL,	SE,	MC,	P1
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL	, TR,	BG,	CZ,	EE,	HU,	SK	
BR	2003	0089	74		A		2005	0215		BR	2003-	8974			2	0030	402
US	2005	0905	02		A1		2005	0428		US	2003-	5100	26		2	0030	402
CN	1646	508			Α		2005	0727		CN	2003-	8078	87		2	0030	40
JΡ	2005	5355	68		T		2005	1124		JΡ	2003- 2003- 2003- 2003-	5803	08		2	0030	402
NO	2004	0047	45		А		2004	1214		NO	2004-	7,43			-	0041	10,
RITY	APP	LN.	INFO	.:						US	2002-	3697	79P		P 2	0020	40:
										US	2002-	3699	30P		₽ 2	0020	40:
										wo	2003-	EP34	66	,	w 2	0030	402

OTHER SOURCE(S): MARPAT 139:307766

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Substituted thiazolidinetriones I (L1 = L2 = single bond; O1 = single bond, H, (un)substituted alkyl, cycloalkyl, or aminocarbonyl, carboxy, RlOC(:O), RlOC(:O), RlOC(:O), RlOS(:O)q; O2 = O, S, RRN; R, R2 = (un)substituted alkyl, alkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, or aralkylthio, amino, halogen, nitro, carboxy, trifluoromethyl, etc.; Rl = (un)substituted alkyl, aryl, heteroaryl, aralkyl, RlO = (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaryl, RlO = (un)substituted alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl; RlO = (un)substituted alkyl, aryl, betwooryl, acyl, aryloxycarbonyl, heteroaryloxycarbonyl, carbamoyl, or sulfonyl; X, Y = CH, N, O, 5, RlAN; Z = (un)substituted alkyl, alkoxyalkyl, alkylthioalkyl, alkylaminoalkyl; 2l, ZZ, ZZ = CH, N, N(:O), CRl, CR2; Rl and R2 can form an (un)substituted 5 - or 6-membered aromatic or heteroarom. ring; Rl and Ll can form an (un)substituted 5-,

r 7-membered ring interrupted by nitrogen, oxygen or sulfur atoms) such as II are prepared as inhibitors of protein tyrosine phosphatase 1b and

protein tyrosine phosphatase for overcoming insulin resistance and modulating glucose levels in the treatment or prevention of metabolic diseases, such as diabetes, or atherosclerosis. II is prepared by

.men. of Et bromoacetate with 1-naphthalenemethanamine, N-sulfamoylation with sulfamoyl chloride, and base-mediated cyclocondensation. No biol. data

IT

provided.
612530-89-8P 612530-90-2P 612530-92-4P 612530-83-5P 612530-94-6P 612530-92-4P 612530-93-5P 612530-93-6P 612530-93-6P 612530-93-6P 612531-00-7P 612531-00-8P 612531-00-9P 612531-00-9P 612531-00-9P 612531-10-9P 612531-13-2P 612531-22-3P 612531-13-4P 612531-31-4P 612531-32-5P 612531-31-7P 612531-31-5P 612531-31-69P 612531-61-0P 612531-66-5P 612531-61-0P 612531-66-5P

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-92-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[(2,4-dimethoxypheny])methyl]-5-[(4-methoxy7-quinolinyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612531-67-69 612531-68-79 612531-69-89
612531-70-1P 612531-75-69 612531-72-39
612531-77-49 612531-75-69 612531-76-79
612531-77-69 612531-78-99 612531-79-0P
612531-69-03P 612534-94-89
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of thiazolidinetriones as protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosalerosis)
612530-69-9 HCAPLUS
Carbamic acid, [4-[(5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612530-90-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 2-{(2,4-dimethoxyphenyl)methyl]-5-{(1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612530-94-6 HCAPLUS

Of Servic acid,
4-([5-([2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, [4-(methylsulfonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (C

(Continued)

PAGE 2-A

IN 612530-95-7 HCAPLUS
IN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(bromomethyl)phenyl)methyl]-2-[(2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-

RN 612530-98-0 HCAPLUS
CN Acetic acid, [[[4-[[5-{(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-chladiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

RN 612530-96-8 HCAPLUS
Acetic acid, [[[4-[[5-[(2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

.

RN 612530-99-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-iodophenyl)methyl]-2-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-00-7 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl], phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-01-8 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl}-3-[[5-[(4-

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-05-2 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-10-9 HCAPLUS

Benzaldehyde,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-02-9 HCAPLUS
CN Carbamic acid,
[(1S)-1-{[3-[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-2-oxo-2(pentylamino)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612531-03-0 HCAPLUS Benzenepropanamide, α -amino-3-[[5-[{4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl}-N-pentyl-, (α S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 'ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

·612531-13-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612531-22-3 HCAPLUS
CN Carbamic acid, [{4-[5-[{2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo1,2,5-chiadiacolidin-2-yl]methyl)phenyl}methyl}-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612531-23-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2 | OMe

RN 612531-30-3 HCAPLUS
CN Benzoic acid,
4-{[5-{(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-{aminomethyl)phenyl]methyl}-2-{(2,4-dimethoxyphenyl]methyl}-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

RN 612531-24-5 HCAPLUS
CN Carbamic acid,
[2-{[(4-{[5-{(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl]methyl]phenyl]methyl]amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A | OMe

RN 612531-31-4 HCAPLUS
CN Benroic acid,
4-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-32-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, [4-((1,1-dimethylethoxy)carbonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-35-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-2-{(2,4-dimethoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-36-9 HCAPLUS
Benzoic acid, 3-[5-[(2,4-dimethoxyphenyl)methyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yll-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 2-A

612531-34-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{2,4-dimethoxyphenyl)methyl}-5-(2,4-dinitrophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612531-61-0 HCAPLUS
1H-1,4-Benzodiazepine-2,5-dione, 3-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-(phenylmethoxy)phenyl]methyl]-3,4-dihydro- (9CI)
(CA INDEX NAME)

RN 612531-63-2 MCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-2-(1(4-methoxyphenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-64-3 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-65-4 HCAPLUS CN D-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, phenylaethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-68-7 HCAPLUS
CN Benzenepropananide, a-amino-4-[5-[(4-methoxyphenyl)methyl]-1,1dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612531-69-8 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-[5-[{4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-66-5 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-4-{5-{(4-methoxphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-67-6 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-70-1 HCAPLUS
CN L-Phenylalanine, 4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-71-2 HCAPLUS
CN L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-[(4-methoxyphenyl)methyl]1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-72-3 HCAPLUS
CN L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-[(4-methoxyphenyl)methyl)1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-73-4 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-[2-(1,1-dimethyy)-2-oxoethyl]phenyl]ethyl]-4-[5-[(4-methoxyphenyl)methyl]-1,l-dloxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-77-8 HCAPLUS CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl}-3-[5-[(4-methoxyphenyl)]-nethyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-78-9 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-3-{5-{4-methoxyphenyl}methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-75-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-76-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-2-([(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (C

(Continued)

RN 612531-79-0 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiacolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl)-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-80-3 HCAPLUS
CN Benzenepropanamide, α-amino-3-[5-[{4-methoxyphenyl}methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-, {αS}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612534-94-8 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[5-[(4-...methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612527-93-2P 612530-46-8P 612530-49-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) , (invention compound; preparation of thiazolidinetriones as protein size.

phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis) 612527-33-2 MCARUS

1,2,5-Thiadiazolidin-3-one, 5-[(3-aminophenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 612527-98-79 612527-99-89 612528-00-4P 612528-01-5P 612528-02-6P 612528-07-1P 612528-01-6P 612528-01-6P 612528-10-6P 612528-11-7P 612528-12-8P 612528-13-9P 612528-11-7P 612528-18-4P 612528-13-9P 612528-13-9P 612528-11-7P 612528-18-4P 612528-19-5P 612528-13-9P 612528-13-9P 612528-23-9P 612528-33-9P 612528-33-9P 612528-33-9P 612528-34-2P 612528-34-2P 612528-34-39-9P 612528-34-2P 612528-34-39-9P 612528-34-2P 612528-34-3P 612528-35-3P 612528-55-3P 612528-35-3P 612528-56-2P 612528-35-3P 612528-66-2P 612528-66-2P 612528-67-3P 612528-75-3P 612528-39-3P 6

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-46-8 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
ester (9C1) (CA INDEX NAME)

612530-49-1 HCAPLUS Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, methyl ester (9CI) (CA IMDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 612530-04-8P 612530-05-9P 612530-06-0P 612530-00-2P 612530-09-3P 612530-10-6P 612530-11-7P 612530-12-8P 612530-13-9P 612530-16-2P 612530-17-3P 612530-18-4P 612530-22-0P 612530-23-1P 612530-23-9P 612530-22-0P 612530-23-1P 612530-23-1P 612530-23-1P 612530-23-1P 612530-27-5P 612530-23-1P 612530-33-3P 612530-31-1P 612530-33-5P 612530-33-9P 612530-31-1P 612530-33-9P 612530-33-5P 612530-34-6P 612530-33-5P 612530-44-6P 612530-45-7P 612530-43-5P 612530-40-6P 612530-45-9P 612530-40-6P 612530-45-5P 612530-46-0P 612530-60-6P 612530-61-5P RL: PAC (Pharmacological activity): SPN (Synthetic p (Continued) RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES ses) (invention compd.; prepn. of thiazolidinetriones as protein tyrosine phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or

mitigate insulin resistance in the treatment of diabetes of atherosclerosis) 612527-84-1 RCAPLUS 1,2,5-Thiaddazolidin-3-one, 5-(1-naphthalenylmethyl)-, 1,1-dioxide (9CI)

(CA INDEX NAME)

612527-85-2 HCAPLUS
Acetamide, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-86-3 HCAPLUS
Carbamic acid, [[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612527-87-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612527-88-5 HCAPLUS
Acetamide, N-[[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1]pheny1]methy1]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-91-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-iodophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-92-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-94-3 HCAPLUS
Acetamide, N-{3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-89-6 HCAPLUS
Carbamic acid, [[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

612527-90-9 HCAPLUS
Benzenepropanamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl}- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612527-96-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-aminophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-97-6 HCAPLUS
Butanamide, N-[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}phenyl]- (9CI) (CA INDEX NAME)

RN 612527-98-7 HCAPLUS Urea, N- $\{3-\{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl\}methyl\}phenyl}-N'-$ 612527-98-7 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN propyl- (9CI) (CA INDEX NAME) (Continued)

612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

612528-00-4 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9CI) (Cd IMDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-07-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(4-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-08-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(4-amino-2-bromophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-09-3 HCAPLUS
Acetamide, N-{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}phenyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-01-5 HCAPLUS
Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl](9CI) (CA INDEX NAME)

RN 612528-02-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methylphenyl)methyl]-, 1,1-dioxide
(9CI)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-10-6 HCAPLUS Metheneulfonamide, N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

612528-11-7 HCAPLUS
Methanesulfonamide, N-[[4-[[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-12-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methylphenyl)methyl}-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612528-13-9 HCAPLUS
CN Benzeneacetic acid, α-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-14-0 HCAPLUS
CN Benzeneacetamide, α-amino-2-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-15-1 HCAPLUS
CN Benzeneacetamide, q-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-16-2 HCAPLUS Benzeneacetamide, 4-[(1,1-dioxido-4-ox-1,2,5-thiadiazolidin-2-y1)methyl]- N-propyl- α -[(trifluoroacety1)amino]- (9CI) (CA INDEX NAME)

RN 612528-17-3 HCAPLUS
CN Benzeneacetamide,
4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}a-((methylsulfonyl)aminol-N-propyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continu

RN 612528-18-4 HCAPLUS
CN Benzenepropanamide, α-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-19-5 HCAPLUS
CN Propanedioic acid, (acetylamino)[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 Of 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-20-8 HCAPLUS
CN Benzenepropanamide, α-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-21-9 HCAPLUS
CN Phenylalanine, N-acetyl-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-26-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(2-chlorophenyl)ethyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

RN 612528-27-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(4-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-22-0 HCAPLUS CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-23-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-25-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3,4-dimethoxyphenyl)ethyl]-,
1,1-dioxide
(SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-28-6 HCAPLUS CN Acetamide, N-[4-[2-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)ethyl]phenyl]-2,2,2-trifluoro-(9CI) (CA INDEX NAME)

RN 612528-29-7 HCAPLUS
CN Butanamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-32-2 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-α-(phenylmethyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-33-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

.

(Continued)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 5-yl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-37-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methoxy-7-quinolinyl)methyl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-38-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(2-methylpropoxy)-7-quinolinyl]methyl]-, 1.1-dioxide (9CI) (CA INDEX NAME)

RN 612528-39-9 HCAPLUS Glycine, N-[2-(butylsmino)-2-oxo-1-phenylethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadizolidin-2-yl]methyl]benzoyl]- (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-34-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{{4-(aminomethyl)-1-naphthalenyl}methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-35-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{{1-ethyl-2-methyl-1H-benzimidazol-5-yl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-36-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-methyl-1-(3-methylbutyl)-1H-benzimidazol-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-40-2 HCAPLUS
CN Glycine, N-[2-(butylamino)-1-(4-ethylphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continu

PAGE 2-

RN 612528-41-3 HCAPLUS
CN Glycine, N-[2-(butylamino)-2-oxo-1-(3-phenoxyphenyl)ethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612528-42-4 HCAPLUS
CN Glycine, N-[2-(butylamino)-1-(4-methoxyphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-

PAGE 2-A

RN 612528-44-6 HCAPLUS Glycine, N-[2-{butylamino}-1-{2-naphthalenyl}-2-oxoethyl}-N-{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}benzoyl}- (9CI) (CA INDEX NAME)

RN 612528-45-7 HCAPLUS Glycine, N-[2-(butylamino)-1-(4-chlorophenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1-2,5-thiadiarolidin-2-yl)methyl]benzoyl]- (SCI) (CA INDEX

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612528-43-5 HCAPLUS
CN Glycine, N-[1-(2-bromophenyl)-2-(butylamino)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued , NAME)

PAGE 1-A

PAGE 2-A

RN 612528-46-8 HCAPLUS
CN Glycine, N-[2-(butylamino)-2-oxo-1-[3-(phenylmethoxy)phenyl]ethyl]-N-[4[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA
INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued) PAGE 1-A

PAGE 2-A

RN 612528-47-9 HCAPLUS
CN Glycine,
N-(12E)-1-[(butylamino)carbonyl]-3-phenyl-2-propenyl]-N-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 612528-48-0 HCAPLUS CN Glycine, N-[1-[(buylamino)carbony1]-3-phenylpropy1]-N-[4-[(1,1-dioxido-4-

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) PAGE 2-A

612528-50-4 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(3-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 1-A

612528-51-5 RCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-butylphenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-49-1 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
[4-(methylsulfonyl)phenyl]methyl ester {9Cl} (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612528-52-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(hydroxymethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

PAGE 2-A

612528-53-7 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
{2-(2-phenylethyl)menyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Conti [4-(difluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME) (Continued)

PAGE 2-A

RN 612528-56-0 HCAPLUS
CN 2-Thiopheneacetic acid,
5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl]methyl]benzoyl]oxy]methyl]-a,a-difluoro- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-54-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
[1,1'-biphenyl]-2-ylmethyl ester (9CI) (CA INDEX NAME)

612528-55-9 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-57-1 HCAPLUS Acetic acid, [[[4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]sulfonyl]-, ethyl ester [9CI) (CA INDEX NAME)

612528-58-2 HCAPLUS
Acetic acid, [[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y]]hethyl]phenyl]phenyl]phenyl]sethyl]thio]-, ethyl ester [9C1] (CA INDEX NAME)

RN 612528-59-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(3-methylbucyl)thio]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Me2CH-CH2-CH2-S-CH2

612528-60-6 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-ethylbutyl ester (9CI) (CA INDEX NAME)

612528-61-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclobutylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-64-0 HCAPLUS
Benzoic acid, 4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2,4,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

о- cн₂-сн-сн₂-сме₃

612528-65-1 MCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,cyclohexylmethyl ester (9C1) (CA INDEX NAME)

612520-66-2 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612520-62-8 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, cyclopentylmethyl ester (9CI) (CA INDEX NAME)

612528-63-9 HCAPLUS
Benzoic acid, 4-[(1],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,2-methylpentyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-67-3 RCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclopentyl ester (9CI) (CA INDEX NAME)

612528-68-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-methylbyl ester (9CI) (CA INDEX NAME)

612528-69-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-,
2-(methylthio)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-70-8 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-[(carboxymethyl)thio]ethyl ester (9CI) (CA INDEX NAME)

NN 612528-71-9 HCAPLUS
NB Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(5-nitro-2-furanyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2-OH

RN 612528-74-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[3-(methylsulfonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-72-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-pyridinylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-73-1 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
[3-(hydroxymethyl)phenyl]methyl ester {9Cl} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

PAGE 1-A

PAGE 2-A

RN 612528-75-3 HCAPLUS
CN Benzeneacetic acid, 4-[4-[[4-[[4,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]amino]butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

PAGE 2-A

612528-76-4 HCAPLUS
Benzeneacetic acid, 4-{3-{(4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y)|methyl|benzoyl|amino|propyl|- {9C1} (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

(Continued)

PAGE 2-A

612528-77-5 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[5-{(dimethylamino)methyl}-2-furanyl}methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-78-6 HCAPLUS L-Phenylalaninamide, .N-acetyl-L-phenylalanyl-3-{(1,1-dioxido-4-oxo-1,2,5-thadiazolidin-2-yl)methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612528-79-7 HCAPLUS
1,2,5-Thladiazolidin-3-one, 5-(1H-indol-5-ylmethyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612528-80-0 HCAPLUS
1,2,5-Thladiazolidin-3-one, 5-[(3,4,5-trimethoxyphenyl)methyl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

612528-82-2 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 5-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-83-3 RCAPLUS Bernzenecetic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl|- (9C1) (CA INDEX NAME)

612528-84-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-benzoylphenyl)methyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-85-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-86-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(4-methyl-1-oxopentyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612528-89-9 HCAPLUS CN 2(1H)-Quinolinone, 6-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

612528-97-9 HCAPLUS
Acetamide, 2-amino-N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]pheny1]methy1]- (9CI) (CA INDEX NAME)

612528-98-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(4-carboxyphenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-87-7 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-[[3-(2-fluorophenoxy)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612528-88-8 HCAPLUS
Benzoic acid, 3-[2-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]ethoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

612528-99-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-phenoxyphenyl)methyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-00-7 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-y1)methyl]-3-nitro- [9CI] (CA INDEX NAME)

612529-01-8 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[[4-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-02-9 RCAPLUS
Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-05-2 HCAPLUS
Benzoic acid, 5-amino-2-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}- (9CI) (CA INDEX NAME)

RN 612529-06-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-methoxy-5-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-03-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-hydroxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-04-1 HCAPLUS
Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-5-nitro- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 61252-07-4 HCAPLUS 1,2,3-Thiadiarolidin-3-one, 5-{(2-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-08-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-methyl-2-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-09-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-methylphenyl)methyl}-, 1,1-dioxide

(CA INDEX NAME)

612529-10-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-phenylpropyl)-, 1,1-dioxide (9CI) (CA

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) INDEX NAME)

RN 612529-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-butoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

H N CH2

RN 612529-12-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

H N S CH2

- RN 612529-13-2 HCAPLUS
 CN Benzoic acid, 3-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]- (9CI) (CA INDEX NAME)
- L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

H OON CH2

RN 612529-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methyl-3-nitrophenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

H N O

RN 612529-17-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(5-methyl-2-nitrophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-18-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-aminophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

H_N CH₂ CH₂

RN 612529-14-3 HCAPLUS
CN Benzenebutanoic acid,
5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)- (9CI) (CA INDEX NAME)

HO2C-(CH2)3

RN 612529-15-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methyl-3-nitrophenyl)methyl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

H₂N CH₂

RN 612529-19-8 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin_-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

O CH2-N NH

RN 612529-20-1 HCAPLUS CN 1H-Isoindole-1,3(2H)-dione, 2-{[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

CH2 CH2 NH

RN 612529-21-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[1,4-phenylenebis(methylene)]bis-, 1,1,'1,'t-tervoxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-22-3 HCAPLUS CN Acetic acid, [[2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)methyl]phenyl]aminoloxo- (9CI) (CA INDEX NAME)

RN 612529-23-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, S-[(3-hydroxyphenyl)methyl]-, 1,1-dioxida (9CI) (CA INDEX NAME)

RN 612529-24-5 HCAPLUS
CN Benzoic acid, 2-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-28-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-amino-5-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-29-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-4-methylphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-30-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-amino-3-methylphenyl)methyl}-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-26-7 HCAPLUS CN 1,2,5-Thiaddazolidin-3-one, 5-[[4-fluoromethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

14 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (C

RN 612529-31-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-2-methylphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-32-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-5-methylphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-33-6 HCAPLUS
CN Acetamide, N-[{4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]methyl]-2,2,2-trifluoro-(9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612529-37-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-hydroxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-41-6 HCAPLUS
CN Benzoic acid, 2-amino-5-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-42-7 HCAPLUS
CN Benzoic acid,
2-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-43-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-(phenylmethyl)phenyl]methyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-38-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, S-[(3,5-dimethylphenyl)methyl]-, 1,1-dioxide
(901) (CA INDEX NAME)

RN 612529-39-2 HCAPLUS
CN L-Phenylalanine, N-{[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl}methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-40-5 HCAPLUS
CN L-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-44-9 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one, 5-[[2,4-bis(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4,6-trifluorophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-46-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-bromophenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-47-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5,5'-[[1,1'-biphenyl]-2,2'-diylbis(methylene)]bis-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

612529-48-3 KCAPLUS
1,2,5-Thiadiacolidin-3-one, 5-[[4-[[ethylamino]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-49-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Ph-CH2-CH2-NH-CH2

612529-52-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-{(diethylamino)methyl}phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-53-0 HCAPLUS
Benzoic acid, 22-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl|-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid,
2-(acetylamino)-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}- (9CI) (CA INDEX NAME)

612529-50-7 HCAPLUS
Benzoic acid, 2-amino-4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}-, ethyl ester (9CI) (CA INDEX NAME)

RN 612529-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(2-phenylethyl)amino]methyl]phenyl]met
hyl]-, 1,1-dioxide (9CI). (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-54-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 612529-56-3 HCAPLUS
CN Benzamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[2-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612529-57-4 HCAPLUS
CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(3-methylbutyl)- (9CI) (CA INDEX NAME)

RN 612529-58-5 HCAPLUS CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-a-(phenylmethyl)-, 1,1-dioxide; (us)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 612529-59-6 HCAPLUS
CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo-α-(phenylmethyl)-,
1,1-dioxide, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-63-2 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-64-3 HCAPLUS CN Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)methyl]phenoxyl-, methyl ester (9C1) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-60-9 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

RN 612529-61-0 HCAPLUS CN Acetic acid, [4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)methyl]phenoxyl- (SCI) (CA INDEX NAME)

RN 612529-62-1 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-65-4 HCAPLUS
CN Benzoic acid, 4-[(l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(carboxymethoxy)phenyl]methyl ester (9C1) (CA INDEX NAME)

PAGE 1~A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612529-67-6 HCAPLUS
Benzoic acid, 4-(2-([(4-((),1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y))methyl]phenyl]methyl]aminojethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

(Continued) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-73-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

612529-74-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, ethyl ester (9C1) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue 612529-68-7 HCAPLUS Acetic acid, (4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenoxy]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

(Continued)

612529-69-8 HCAPLUS
Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenoxy]-, phenylmethyl ester (9CI) (CA INDEX NAME)

612529-70-1 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-75-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-76-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-ethoxyphenyl)methyl]-, 1,1-dioxide
(9CI) /

(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2

RN 612529-77-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[3-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-78-9 HCAPLUS
CN Benzeneacetic acid, 4-{{{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1}benzoy1}oxy}methy1}- {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-80-3 MCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-(phenylamino)ethyl ester (9CI) (CA INDEX NAME)

RN 612529-81-4 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-{3-methoxyphenyl}ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612529-79-0 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-phenylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-F

RN 612529-82-5 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl
ester (9CI) (CA INDEX NAME)

RN 612529-83-6 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2,2-dimethylpropyl ester {9CI} (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-84-7 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-methoxy-2,2-dimethyl-3-oxopropyl ester (9CI) (CA INDEX NAME)

RN 612529-85-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2,2,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-90-5 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
(3-methyl-4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 1-A

612529-91-6 HCAPLUS
8 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-86-9 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-(dimethylamino)-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-87-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[(3aR,4s,5R,6aS)-5-(benzoyloxy)hexahydro-2-oxo-2H-cyclopenta[b]furan-4yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (3-chloro-4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612529-93-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
6-ethoxy-6-oxohexyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-94-9 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(3-chlorophenyl)ethyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-[3-(trifluoromethyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

612529-97-2 HCAPLUS
D-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)phenyl]methyl}-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612529-98-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[(phenylmethyl)amino]methyl]phenyl]meth

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612529-95-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-(3-methylphenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

PAGE 1-A

612529-96-1 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN y1}-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

612529-99-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612530-01-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
[4-(methoxycarbonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612530-03-7 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-phenoxypropyl ester (9CI) (CA INDEX NAME)

612530-04-8 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[4-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612530-02-6 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-cyclohexyl-2-methylpropyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 2-A

612530-05-9 HCAPLUS
Benzoic acid, 4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[3-(trifluoromethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

612530-06-0 HCAPLUS
Benzoic acid, 4-{(i,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-(4-carboxyphenyl)ethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

DAGE 2-

N 612530-08-2 HCAPLUS N Benzoic acid, 3-[[[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

i-BuNH-CH2

RN 612530-10-6 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one,
5-[[4-[(2.2-dimethyl]propyl)amino]methyl]pheny
1]methyl)-, 1.1-dioxide (9CI) (CA INDEX NAME)

Me3C-CH2-NH-CH2

RN 612530-11-7 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
1-naphthalenylmethyl ester (9CI) (CA INDEX NAMÉ)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

со2н

RN 612530-09-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[{4-[((2-methylpropyl)amino]methyl]phenyl]me thyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (C

(Continued)

PAGE 1-A

PAGE 2-A

NN 612530-12-8 HCAPLUS
NN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

DACE 2-

N 612530-13-9 HCAPLUS
N Benzeneaccia acid, 4-[2-{[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]amino|ethyl}- (9Cl) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

DACE 1-7

PAGE 2-A

(Continued)

NO;

RN 612530-17-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-[(carboxymethyl)amino]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-18-4 HCAPLUS

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612530-16-2 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

RN 612530-19-5 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-,
(1,1'-biphenyl]-4-ylmethyl ester (9C1) (CA INDEX NAME)

CH2

PAGE 2-A

PAGE 1-A

RN 612530-20-8 HCAPLUS

- ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
 [4-(acetylamino)phenyl]methyl ester (9CI) (CA INDEX NAME)
 - PAGE 1-A

PAGE 2-A

$$\Diamond$$

- 612530-21-9 HCAPLUS
 Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
 [2-(phenylmethyl)phenyl]methyl ester (9C1) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (2-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

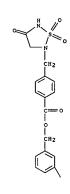
- 612530-25-3 HCAPLUS
 Benzeneacetic acid, 3-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- 612530-22-0 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
 (2-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

- 612530-23-1 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
- L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

- 612530-26-4 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
 (4-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

612530-27-5 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
[4-fluoro-2-(trifluoromethyl)phenyl}methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-B

612530-29-7 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI)
(CA INDEX NAME)

612530-30-0 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(5-methyl-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

RN 612530-28-6 HCAPLUS
CN Benzoic acid,
4-[{5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]lmethyl]-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

(Continued)

PAGE 2-A

612530-31-1 HCAPLUS
Benzoic acid, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylphenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

RN 612530-32-2 HCAPLUS
CN Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
3-((carboxymethyl)methylamino)-2,2-dimethylpropyl ester (9CI) (GA INDEX NAME)

RN 612530-33-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)-,
phenyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-37-7 HCAPLUS
CN 1-Piperazineacetic acid, 4-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]- (9CI) (CA INDEX NAME)

RN 612530-38-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-34-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-[(2-methyl)propyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA
INDEX NAME)

RN 612530-35-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenylmethyl ester (9CI) (CA INDEX NAME)

RN 612530-36-6 HCAPLUS
CN Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N,N-bis(2-methylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Cont

RN 612530-39-9 HCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]oxy]methyl]-, 2-methylpropyl ester
(9CI) (CA INDEX NAME)

RN 612530-40-2 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[[5-(aminocarbonyl)-2-thienyl]methyl ester [SCI] (CA INDEX NAME)

RN 612530-41-3 HCAPLUS CN Piperazine, 1-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)benzoyl]-4-[(phenylmethyl)- (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-42-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(1-oxo-3-yhenylpropyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

612530-43-5 HCAPLUS
Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
[5-{{{phenylmethyl}amino}carbonyl}-2-thienyl]methyl escer (SCI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-48-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{4-(aminomethyl)phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-50-4 HCAPLUS Benzeneacetic acid, 2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(CA INDEX NAME)

612530-51-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-dimethoxyphenyl)-, 1,1-dioxide, potassium salt (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-45-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide (9CI) INDEX NAME)

612530-47-9 HCAPLUS Benzoic acid, 3-(1,1-dioxido-4-oxo+1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-52-6P 612530-53-7P 612530-54-8P 612530-55-9P 612530-56-0P 612530-57-1P 612530-58-2P 612530-59-3P 612530-60-6P 612530-61-7P 612530-62-8P 612530-63-9P 612530-64-0P 612530-65-1P 612530-66-2P 612530-67-3P 612530-68-4P 612530-69-5P 612530-71-3P 612530-72-0P 612530-73-1P 612530-73-8P 612530-73-9P 612530-73-1P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 61250-78-6P 612534-93-7P 61250-78-6P 612534-93-7P 612530-73-5P (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (es)

phosphatase 1b and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosolerosis) 612530-52-6 HCAPLUS Acetamide, 2-(4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-methylphenoxy]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

612530-53-7 HCAPLUS
1H-1,4-Benzodiazepine-2,5-dione, 3-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-hydroxyphenyl]methyl]-3,4-dihydro- (9CI) (CA

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)

RN 612530-54-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-55-9 HCAPLUS
CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. .

RN 612530-56-0 HCAPLUS
CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)- (9CI)
(CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

RN 612530-60-6 HCAPLUS
CN L-Phenylalaninamide, N-benzoyl-O-(dicarboxymethyl)-L-tyrosyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-61-7 HCAPLUS
Senzemepropanamide, α-[([1,1'-biphenyl]-4-ylsulfonyl)amino]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl-, (α\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 612530-57-1 RCAPLUS
CN L-Phenylalaninamids, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-58-2 HCAPLUS
CN L-Phenylalaninamids, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiddiazolidin-2-yl)-N-(4-phenylbutyl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-59-3 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-(carboxymethyl)phenyl]ethyl]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612530-62-8 HCAPLUS
CN Benzenepropanamide, α-[([1,1'-biphenyl]-4-ylsulfonyl)amino]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)-, (αS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-63-9 HCAPLUS
CN Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-Npentyl-α-[(phenylsulfonyl)amino]-, (αS)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

RN 612530-64-0 HCAPLUS

Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-(4-phenylbutyl)-\alpha-{(phenylsulfonyl)amino}-, (\alpha S)- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 612530-65-1 HCAPLUS
CN Benzenepropanamide,
4-(1,-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(3,3diphenylpropyl)-a-[(phenylsulfonyl)amino]-, (aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612530-66-2 HCAPLUS
CN L-Phenylalaninamide,
N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-{(4-aminophenyl)methyl}-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 612527-96-5 CMF C9 H11 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612530-72-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(1-ethyl-2-methyl-1H-benzimidazol-5yl)methyl]-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612528-35-5 CMF C13 H16 N4 O3 S

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-67-3 HCAPLUS Benzenepropanamide, 3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- α -([phenylsulfonyl]amino]-, (aS)- [9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-68-4 HCAPLUS
CN L-Phenylalaninamide,
N-acctyl-L-phenylalaninayl-3-bromo-4-(1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-69-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-71-9 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM 2

CRN 76-05-1 CMF C2 H F3 O2

612530-73-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-[(Z)-(3-oxo-2(3H)-benzofuranylidene)methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

612530-74-2 HCAPLUS Ethanedione, {4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]phenyl- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-75-3 HCAPLUS
9,10-Anthracenedione, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1)- (9CI) (CA INDEX NAME)

612530-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide, sodium salt (9CI) INDEX NAME)

● Na

612530-78-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide, trifluoracetate (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (CONTINUED)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

CM 1

CRN 612530-45-7 CMF C8 H10 N4 O3 S

CM 2

612534-93-7 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 31 Jul 2002
ACCESSION NUMBER: 2002:565367 HCAPLUS
DOCUMENT NUMBER: 137:232603
TITLE: AUTHOR(S): Efficient Solid-Phase Synthesis of Sulfahydantoins
Tremblay, Melanie: Voyer, Normand; Boujabi, Sihem;
Dewynter, Georges F.
Centre de Recherche sur la Fonction, la Structure et l'Ingenierie des Proteines, Departement de Chimie,
Faculte des Sciences et de Genie, Universite Laval,
Quebec, QC, GIK 7P4, Can.
Journal of Combinatorial Chemistry (2002), 4(5),
429-435
CODEN: JCCHPF; ISSN: 1520-4766
American Chemical Society
Journal
English
OTHER SOURCE(S): CASREACT 137:232603

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB A novel solid-phase strategy allows the efficient preparation of traceless sulfahydantoins. A total of 28 derivs., with crude purity generally higher than 85%, were prepared by parallel synthesis. Through reductive alkylations, Mitsunobu reactions, and sulfamoylation reactions on oxime resim, the synthetic strategy affords sulfahydantoin derivs. selectively substituted at N2, e.g., I, N5, e.g., II, and N2, N5, e.g., III, positions, although yields of disubstituted compds. are lower. The mild reaction conditions involved, lead to sulfahydantoins without racemization.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
459831-33-5P 459831-34-6P 459831-35-TP
RL: SPN (Synthetic preparation) PREP (Preparation)
(stereoselective preparation of N2,N5-disubstituted sulfahydantoins

reductive alkylation of resin-bound phenylalanine with substituted benzaldehydes and subsequent sulfamoylation, Mitsunobu reaction, resin-cleavage, and cyclization)
459831-33-5 HCAPUUS
1,2,5-Thiadiazolidin-3-one,
4-methylphenyl)methyl)-4-(phenylmethyl)-2(2-propenyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-34-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-butyl-5-[(4-methylphenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 459831-35-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methylphenyl)methyl)-4-(phenylmethyl)-2(3-phenylpropyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR

REFERENCE COUNT: THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 33 MCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 283587-14-4P 459831-30-2P 459831-31-3P 459831-32-4P RL: SPN (Synthetic preparation); PREP (Preparation) (stereosalective preparation of N5-substituted sulfahydantoins via ctive
alkylation of resin-bound phenylalanine with substituted benzaldehydes
and subsequent sulfamoylation, resin-cleavage, and cyclization)
283587-14-4 HCAPLUS
1,2,5-ThiadiaTolidin-3-one,

Absolute stereochemistry.

5-[{4-methoxyphenyl]methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

459831-30-2 HCAPLUS Benzonitrile, 4-[([3S]-1,1-dioxido-4-oxo-3-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-31-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-nitrophenyl)methyl]-4-(phenylmethyl)-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-32-4 HCAPLUS 43361-32-4 (phenylmethyl)-, 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSMER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 Oct 2001
ACCESSION NUMBER: 2001:735235 HCAPLUS
DOCUMENT NUMBER: 136:85785
TITLE: A one-step protocol for the N-chloromethylation of heterocyclic imides
AUTHOR(S): He, Shu: Yu, Hongyi: Fu, Qinghong: Kuang, Rongze;

CORPORATE SOURCE:

PUBLISHER

Jeff B.: Groutas, William C.

PORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA

RCE: Synthetic Communications (2001), 31(20), 3055-3058

CODEN: SYNCAV: ISSN: 0039-7911

MARCEL Dekker, Inc.

UMENT TYPE: Journal

GUAGE: English

A convenient single step methodol. for the N-chloromethylation of heterocyclic imides using a mixture of formaldehyde sodium bisulfite uct

and thionyl chloride is described. For example, the chloromethylation of 5-Butyl-3-propyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide gave. 387859-83-8 387859-86-1 RACT (Reactant or reagent) (preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 387859-83-8 HCAPIUS 1,2,5-thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 387859-86-1 HCAPLUS CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-{phenylmethyl}-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9P 387859-88-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 300553-65-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

387859-88-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 5-(chloromethyl)-4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (SCI) (CA IN (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [{1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]{methylsulfonyl}-, butyl ester (9CI) (CA INDEX NAMEL

RN 220869-14-7 HCAPLUS
CN Carbamic acid,
[2-{[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-chiadiazolidin-2-yl]methyl](methylaulfonyl)amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

RN 220869-16-9 HCAPLUS

CN Carbamic acid, [2-[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 13 Jun 2001 ACCESSION NUMBER: 2001:426029 HCAPLUS DOCUMENT NUMBER: 135:282665

DOCUMENT NUMBER: TITLE: 135:282665 Inhibition of serine proteases by functionalized sulfonamides coupled to the

1, 2, 5-thiadiazolidin-3-one

ne
1,1 dioxide scaffold
Groutas, W. C.; He, S.; Kuang, R.; Ruan, S.; Tu, J.;
Chan, H.-K.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (2001), 9(6),
1543-1548 AUTHOR (5):

CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd. PURLISHER:

DOCUMENT TYPE: LANGUAGE: AB A challeng

NGG: IFF: Jouinal WGG: English A challenge associated with drug design is the development of selective inhibitors of proteases (serime or cysteine) that exhibit the same

1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold yields potent, time-dependent inhibitors of the serine proteases human leukocyte elastase

(HLE), proteinase 3 (PR 3) and cathepsin G (Cat G). Our preliminary findings suggest that (a) appending to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold recognition and diversity elements that interact with both the S and S' subsites of a target protease may result in optimal enzyme selectivity and potency and, (b) functionalized sulfonamides constitute a powerful design and diversity element with low intrinsic chemical reactivity and potentially wide applicability. Potent inhibitors of human leukocyte elastase, proteinase 3 and cathepsin G that interact with the S and S' subsites are realized by using functional sulfonamides coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold.

17 200869-05-6F 200869-07-8P 200869-01-47P 200869-01-47P 365216-42-9P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified): PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (inhibition of serine proteases by functionalized sulfonamides coupled to 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)

RN 20089-05-6 HCAPLUS
CN Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]-2-oxoethyl]-, phenylmethyl ester (SCI) (CA INDEX NAME)

365216-39-3 HCAPLUS

RN 365216-39-3 HCAPLUS
CN Benzamide,
N-[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5thiadiazolidin-2-yl]methyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

365216-41-7 HCAPLUS

Glycine,
{{ [{-(2-methylpropyl)-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5thiadiazolidin-2-yl]methyl]{methylsulfonyl}amino}carbonyl}-, ethyl ester
{9CI (CA INDEX NAME)

365216-42-8 HCAPLUS

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, butyl ester (9CI) (CA
INDEX
NAME)

RN 365216-43-9 HCAPLUS
CN L-Phenylalanine, N-[[[[(45)-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-

(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl] {methylsulfonyl) amino}carb onyl}-, methyl ester (9CI) {CA INDEX NAME}

Absolute stereochemistry.

REFERENCE COUNT: THIS there are 35 cited references available for

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 283587-15-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((2,4-dichlorophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-16-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[(3-methylphenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-18-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[{4-(trifluoromethyl)phenyl]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 24 Apr 2001
ACCESSION NUMBER: 135:76831
TITLE: SAUTHOR(S): Albericio, Fernando; Bryman, Lois M.; Garcia, Javier, Michelotti, Enrique L.; Nicolas, Ernesto; Tice, Colin M.

CORPORATE SOURCE: Department of Organic Chemistry, University of Barcelona, 8arcelona, 08028, Spain Journal of Combinatorial Chemistry (2001), 3(3), 290-300
CODDN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
Journal English
COTHER SOURCE(S): CASREACT 135:76831
AB A five-step solid-phase synthesis of sulfahydantoins from d-amino acids and aldehydes was developed. The synthetic method allows the use of hindered amino acids, including Val. Phe, and Alb, and use of aromatic aldehydes substituted with electron-withdrawing and -donating groups. Some limitations were encountered with amino acids with reactive side chains. A small but diverse library of compds. was produced for biol. testing.

IT 283587-14-4P 283587-15-5P 283587-16-6P 283587-18-9P 283587-12-9P 283587-19-9P 346697-39-0P 346697-3-9-0P 346697-3-9-0P 346697-3-9-0P 346697-3-9-P 346697-3-

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued I, 2,5-Thiadiarolidin-3-one, 5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl}-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-22-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 283587-24-6 HCAPLUS
CN 1,2,5-Thadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[2(methylthiojethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-35-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-((3-chlorophenyl)methyl)-4-(1-methylethyl)-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-36-7 HCAPLUS CN Acetamide, N-[4-[([35)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-37-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(1-methylethyl)-5-(16-nitro-1,3-benzodioxol5-yl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-42-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[[4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (43)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-43-6 HCAPLUS
Acetamide, N-[4-[[(3S)-1,1-dioxido-4-oxo-3-[[4(phenylmethoxy)phenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-44-7 HCAPLUS CN 1,2,5-Thiaddarolidin-3-one, 5-[(6-nitro-1,3-benzodioxol-5-y1)methyl]-4-[(4-(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (4s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 346697-38-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-39-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-40-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-(1-methyl-thyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-41-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[(4-(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-45-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl)-4-[(4-(phenylmethoxyl)phenyllmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-46-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,4-dimethoxy3-methylphenyl)methyl)-4-[(4(phenylmethoxy)phenyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-47-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-chloropheny1)methy1)-4-[2-(methylthio)ethy1-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

346697-48-1 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl}-4-(2-(methylthiolethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 346697-50-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-{{2-chloro-5-{trifluoromethyl}phenyl]methyl}4-{2-(methylthio)ethyl}-, 1,1-dioxide, {4\$}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
346697-55-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-((6-nitro-1,3-benzodioxol-5-yl)methyl)-4[([phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-56-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4[{(phenylmethyl)thio]methyl}-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-chlorophenyl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-58-3 HCAPLUS 1,2,5-Thindiarolidine-3-acetic acid, 2-[[4-(acetylamino)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (38)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-51-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4[[(phenylmethyl)thio)methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

346697-53-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

346697-54-9 HCAPLUS Acetamide, N-[4-[{(3R)-1,1-dioxido-4-oxo-3-[[(phenylmethyl)thio]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid,
2-{(4-chloro-3-nitrophenyl)methyl}-4oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-60-7 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2,4-dimethoxy-3-methylphenyl)methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-62-9 HCAPLUS CN 1,2,5-Thiadiszolidin-3-one, 5-[(4-chlorophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-63-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. .

346697-64-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[3-(trifluoromethyl)phenyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

346697-65-2 RCAPLUS
Benzoic acid, 4-[([35)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-73-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[{2-chloro-5-(trifluoromethyl)phenyl}methyl}4-[{4-(phenylmethoxy)phenyl}methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-74-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-methylphenyl)methyl}-4-{(1-(phenylmethyl)-1H-imidazol-4-yl}methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-75-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-[{1-(phenylmethyl)-1H-imidazol-4-yl}methyl]-

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-69-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[(4-(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-71-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[[4-(phenylmethoxy)phenyl]methyl]-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-72-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[(4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-76-5 HCAPLUS
CN 1,2,5-Thiadiezolidin-3-one,
5-[(2,3-dihydro-1,4-bensodioxin-6-y1)methyl]-4[[1-(phenylmethyl)-1H-imidazol-4-y1]methyl]-, 1,1-dioxide, (45)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

346697-77-6 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-methylphenyl)methyl)-4-oxo-, methyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

RN 346697-79-8 HCAPLUS

L4 ANSMER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(N 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-[[4(trifluoromethyl)phenyl)methyl]-, methyl ester, 1,1-dioxide, (3S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry

RN 346697-80-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4-oxo-, methyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-81-2 HCAPLUS
CN Acetamide, N-[4-[[(3S)-3-[2-(methylthio)ethyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-82-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-(methylthio)ethyl]-5-[(6-nitro-1,3-benzodioxol-5-yl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-86-7 RCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2-chlorophenyl)methyl]-4-oxo-,
phenylmethyl setter, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(4-chlorophenyl)methyl)-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-88-9 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-([6-nitro-1,3-benzodioxol-5-y1]methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (38)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-83-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chlorophenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

N 346697-84-5 HCAPLUS
N 1,2,5-Thiadiarolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl)-4[[(phenylmethyl)thio|methyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-85-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-89-0 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-90-3 HCAPLUS

N 1,2,5-Thiadiazolidin-3-one, 4-[(phenylmethoxy)methyl]-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-91-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[{phenylmethoxylmethyl}]-5-[[3(trifluoromethyl)phenyl]methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-92-5 HCÁPLUS
Benzoic acid, 4-[[{35}-1,1-dioxido-4-oxo-3-[(phenylmethoxy)methyl}-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-93-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4[(phenylmethoxy)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-97-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) .

RN 346698-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-[(2-(trifluoromethyl)phenyl)methyl), 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-04-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-[[3-(trifluoromethyl)phenyl]methyl], 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-05-3 HCAPLUS
Benzoic acid, 4-[(35)-1,1-dioxido-4-oxo-3-phenyl-1,2,5-thiadiazolidin-2-yl]methyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

346697-99-2 HCAPLUS
Benzoic acid, 4-[{(35)-3-[(4-nitrophenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-00-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl)-4-[(4-nitrophenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346698-06-4 HCAPLUS (ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl)-4-phenyl-1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-12-2 HCAPLUS 1,2,5-Thiadiszolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4-[(1S)-1-methylpropyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

346698-14-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, \$-{(4-methoxyphenyl)methyl}-4-{(15)-1-methylpropyl}-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 47 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Dec 2000
ACCESSION NUMBER: 2000:898004 HCAPLUS
DOCUMENT NUMBER: 114:307088

TITLE: 1,2,5-Thiadiazolidin-3-one 1,1 Dioxide: A Powerful Scaffold for Probing the S' Subsites of (Chymo) trypsin-Like Serine Proteases

AUTHOR(S): Groutas, William C.; Epp, Jeffrey B.; Kuang, Rongre; Ruan, Sumei; Chong, Lee S.; Venkataraman, Radhika; Tu.

Juan: He, Shu; Yu, Hongyi; Fu, Qinghong; Li, Yue He; Truong, Tien M.; Vu, Nga T. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Archives of Biochemistry and Biophysics (2001), 385(1), 162-169 CODEN: ABBIA4; ISSN: 0003-9861 Academic Press

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

LANGUAGE: English

The 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) embodies a motif that allows it to dock to the active site of (chymo)trypsin-like

eases
in a predictable and substrate-like fashion. Consequently, inhibitors
derived from this heterocyclic scaffold interact with both the S and S'
subsites of an enzyme. Exploitation of binding interactions with both

s and S' subsites of a target enzyme may lead to compds. With greatly enhanced enzyme selectivity and inhibitory potency. This preliminary report describes the use of a series of compds. having the heterocyclic scaffold linked to various amino acids to probe the S' subsites of human leukocyte elastase (RLE), proteinase 3 (PR 3), and cathepsin G (Cat G). For comparative purposes, a series of compds. derived from a related scaffold, isothiazolidin-3-one 1,1 dioxide (II), was also generated. Several of the compds. were found to be highly potent and selective time-dependent inhibitors of RLE, PR 3, and Cat G. (c) 2001 Academic Press.
334975-68-79 334975-69-09 334975-75-6P 334975-81-4P 334975-88-6P 334975-85-8P RL: BAC (Biological activity or effector, except adverse); BSU

RL: BAC (Biological activity or effector, except adverse); BSU

unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIO: (Biological study); PREP (Preparation) (1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold for probing S' subsites of human leukocyte elastase, proteinase 3 and cathepsin G) RN 334975-68-7 HCAPLUS CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, ((45)-4-(2-methylpropyl]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CRN 76-05-1 CMF C2 H F3 O2

334975-81-4 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

334975-83-6 HCAPLUS L-Phenylalanine, ((45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, monohydrochloride (9CI) (CA INDEX

334975-85-8 HCAPLUS

(Continued) ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

334975-69-8 HCAPLUS
D-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-, [(45)-4-(2-methylproyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-75-6 HCAPLUS
L-Phenylalanine, ((45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 334975-74-5 CMF C23 H29 N3 O5 S

Absolute stereochemistry

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-88-1 HCAPLUS

D-Phenylalanine, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX

CM 1

CRN 334975-87-0 CMF C26 H27 N3 O5 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

THERE ARE 24 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT:

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl-2-oxazolyl)thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS 220037-27-1 mcraus 1/2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-{{(5-phenyl-1,3,4-oxadiazol-2-yl}thio]methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 19 Jul 2000 ACCESSION NUMBER: 2000:488727 HCAPLUS DOCUMENT NUMBER: 133:277919

Potent inhibition of serine proteases by heterocyclic sulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1 dioxide TITLE:

dioxide
He, S.; Kuang, R.; Venkataraman, R.; Tu, J.; Truong,
He, S.; Kuang, R.; Couctas, W. C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic 4 Medicinal Chemistry (2000), 8(7),
1713-1717 AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

DATE OF THE PROPERTY OF THE PR

that the introduction of recognition elements that can potentially interact with the Sn' subsites of these processes might provide an effective means for optimizing enzyme potency and selectivity. Accordingly, a series of heterocyclic sulfide derive, based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) was synthesized and the inhibitory activity and selectivity of these compds. toward human leukocyte elastase (HLE), proteinase 3 (PR 3) and cathepsin G (Cat G) were then determined Compds. with Pl=isobutyl were found to be potent, time-dependent inhibitors of HLE and.

Pl=1sobutyl were found to be potent, time-dependent inhibitors of RLE and, to a lesser extent PR 3, while those with Pl=benzyl inactivated Cat G rapidly and irreversibly. This study has demonstrated that 1,2,5-chiadiazolidin-3-one 1,1 dioxide-based heterocyclic sulfides are effective inhibitors of (chymoltypsin-like serine proteases.

IT 220869-26-1P 220869-27-2P 220869-39-94P 220869-30-7P 220869-310-520 220869-30-7P 220869-310-520 220869-30-7P 220869-310-520 220869-310-8P 220869-30-9P 220869-30-9P 22

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued) 220869-30-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-{(2-benzothiazolylthio|methyl}-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-2-[[(5-phenyl-2-benzoxazolyl)thio]methyl]-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-39-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4,5-bis(phenylmethyl)-2-{((5-phenyl-1,3,4-oxadiazol-2-y))thio]methyl)-, 1,1-dioxide (9CT) (CA INDEX NAME)

220869-40-9 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 2-[[(6-amino-2-benzoxazolyl)thio]methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

$$H_2N$$
 $S-CH_2-N$ CH_2-Ph CH_2-Ph

ΙT

300553-85-9 RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxide derivative; potent inhibition

serine protesses by heterocyclic sulfide derivs. of thiadiszolidinone dioxide)

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 15 Jun 2000 ACCESSION NUMBER: 2000:395930 HCAPLUS DOCUMENT NUMBER: 133:159638

133:159638 Utilization of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold in the design of potent inhibitors

AUTHOR (S):

serine proteases: SAR studies using carboxylates Kuang, R.; Epp. J. B.; Ruan, S.; Chong, L. S.; Venkataraman, R.; Tu, J.; He, S.; Truong, T. M.; Guutas, W. C. Department of Chemietry, Wichita State University, Wichita, KS, 67260, USA Bioorganic & Medicinal Chemistry (2000), 8(5), 1005-1016 CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd.

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

MENT TYPE: Journal
UNGE: English
A series of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one
1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds has been
synthesized and the inhibitory profile of these compds. toward human
leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3) was
then determined Most of the compds. were found to be potent,

then determined Most of the compos. Were sound to septemmed-dependent inhibitors of elastase, with some of the compos. exhibiting kinact/KI values as high as 4,928,300 M-1 s-1. The inhibitory potency of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform was found to be influenced by both the pKs and the inherent structure of the leaving group. Proper selection of the primary specificity group was found to lead to selective inhibition of HLE over Cat G, however, those compds. that inhibited HLE also inhibited PR 3, albeit less efficiently. The predictable mode of binding of these

is. suggests that, among closely-related serine proteases, highly selective inhibitors of a particular serine protease can be fashioned by exploiting subtle differences in their S' subsites. 247179-63-1P 267921-30-6P 287921-33-9P 287921-73-P 267921-38-84 P 287921-33-9P 287921-42-0P 267921-45-3P 287921-56-P 287921-52-P 287921-54-65-PP 287921-591-9P 28

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis of thiadiazolidinone dioxides and isothiazolidinone

as serine protease inhibitors)
247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{{acetyloxy}methyl}-4,5-bis(phenylmethyl}-,
1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

REFERENCE COUNT: THIS

THERE ARE 27 CITED REFERENCES AVAILABLE FOR

RECORD, ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-30-6 HCAPLUS CN Propanoic acid, 2,2-dimethyl-, [4-ethyl-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-33-9 HCAPLUS
Benzeneacetic acid, 4-[[(35)-5-[{2,2-dimethyl-1-oxopropoxy)methyl}-1,1-dioxido-4-oxo-3-propyl-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA

Absolute stereochemistry.

RN 287921-37-3 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[(43)-4-(2-methylpropyl)-1,1-dloxido-3-oxo5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

287921-38-4 HCAPLUS
Benzeneacetic acid, 4-[[(35)-5-[(2,2-dimethyl-1-oxopropoxy)methyl]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI)
(CA INDEX NAME)

287921-39-5 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 2-[(acetyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

287921-42-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(benzoyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenepropanoic acid, {(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX

Absolute stereochemistry

287921-54-4 HCAPLUS
Benzeneacetic acid, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Ph \longrightarrow N \longrightarrow N \longrightarrow N \longrightarrow N$$

RN 287921-65-7 HCAPLUS

Enzoic acid, 2,6-dichloro-,
[(48)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCAPLUS 1,2,5-Thisdiazolidin-3-one, 2-[(acetyloxy)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-45-3 HCAPLUS

Senzoic acid, 2,6-dichloro-,
[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5[phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-46-4 HCAPLUS
Benzeneacetic acid, 4-[{(3S)-5-[{(2,6-dichlorobenzoyl)oxy]methyl}-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

287921-52-2 HCAPLUS

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

212331-98-1P 212331-99-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(aynthesis of thiadiazolidinone dioxides and isothiazolidinone

(synthesis or thrauselesses)
dioxides
as serine protease inhibitors)
RN 212331-98-1 HCAPLUS
CN 1,25-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylthio)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 44 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 19 May 2000 ACCESSION NUMBER: 2000:324184 HCAPLUS DOCUMENT NUMBER: 133:105000

ACCESSION NUMBER: 2000:324184 HCAPLUS
DOCUMENT NUMBER: 133:105000
ITILE: Solid-phase synthesis of sulfahydantoins
AUTHOR(S): Albericio, Fernando; Garcia, Javier; Michelotti,
Enrique L.; Nicolas, Eteneto; Tiec, Colin M.

CORPORATE SOURCE: Department of Organic Chemistry, University of
Barcelona, Barcelona, B8028, Spain

SOURCE: Tetrahedron Letters (2000), 41(17), 3161-3163

COODENT TYPE: Journal
LANGUAGE: English
OOTHER SOURCE(S): CASREACT 133:105000

AB A 5-step solid-phase synthesis of 2-unsubstituted 1,2,5-thiadiazolidin-3one 1,1-dioxides, sulfahydantoins, from No-Famco amino acids and
aromatic aldehydes is described. The key step is the base-mediated
cyclitive

cleavage of a resin bound No-aminosulfonyl No-benryl amino
acid to afford the desired product. This synthesis allows the
preparation of a
diverse library of compds. based on this heterocycle.

IT 281587-14-4P 281587-15-5P 281587-16-6P
281587-18-8P 281587-19-9P 283587-13-PP
283587-18-8P 281587-19-9P 283587-11-9P
283587-18-8P 281587-19-9P 283587-11-9P
283587-18-4P 283587-19-9P 283587-19-9P
281587-18-4P CRAPEUS

CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methoxyphenyl)methyl]-4-(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

283587-15-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-{(4-methoxyphenyl)methyl}-4,4-dimethyl-,1,1-dioxide (9CI) (CA INDEX NAME)

283587-24-6 HCAPLUS
1,2,5-Thiadiszolidin-3-one, 5-[(2-chlorophenyl)methyl)-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 283587-16-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(1-methylethyl)-5-[(3-methylphenyl)methyl]-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 HCAPLUS
1,2,S-Thiadizolidin-3-one, 4-(1-methylethyl)-5-[[4(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (48)- (9CI) (CA INDEX

Absolute stereochemistry.

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

29

THERE ARE 29 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued)

FORMAT

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 27 Aug 1999
ACCESSION NUMBER: 1999:536684 HCAPLUS
DOCUMENT NUMBER: 131:295863
ITILE: 131:295863
AUTHOR(S): Human chymase inhibitors based on the
ITILE: 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold
Groutas, William C.; Schechter, Norman M.; He, Shu;
Yu, Hongyl; Huang, Peng; Tu, Juan
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1999),
9(15), 2199-2204
CODEN: BMCLES; ISSN: 0960-894X
Elsevier Science Ltd.
DOCUMENT TYPE: Lournal
LANGUAGE: English
AB A series of compds. that utilize the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold was synthesized and shown to be highly effective
inhibitors of recombinant human skin chymase.
IT 170918-99-7 247178-61-2 247179-63-1
247179-64-2 247179-68-6 247179-63-7
247179-70-0 247179-71-72-2
247179-71-4 247179-75-5 247179-75-5
EN: BBC (Biological activity or effector, except adverse); BSU
(Biological
study)

R1: BAC (Blological activity of effector, except access, associated);
study, unclassified); PRP (Properties); BIOL (Biological study)
(human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1
dioxide scaffold)
RN 170918-99-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[([4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Acetic acid, hydroxy-,
[{4S}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

RN 247179-66-4 HCAPLUS
CN Propanoic acid, 2-hydroxy-,
[(48)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-67-5 HCAPLUS
Benzeneacetic acid, α-hydroxy-, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1.4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{acetyloxy}methyl}-4,5-bis{phenylmethyl}-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-64-2 HCAPLUS
Propanedioic acid, mono[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-65-3 HCAPLUS

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

247179-68-6 HCAPLUS
1,2,5-Thiadizolidin-3-one, 2-[(methylsulfonyl)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-69-7 HCAPLUS Acetic acid, [[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

247179-70-0 HCAPLUS
Propanoic acid, 3-[[[{45}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

HO₂C

247179-71-1 RCAPLUS
Benzoic acid, 2-[[([45]-1,1-dioxido-3-oxo-4,5-bis(phenylmethy1)-1,2,5-thiadiazolidin-2-y1]methy1]sulfony1}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-72-2 HCAPLUS
Benzoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: THIS

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-74-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

247179-75-5 HCAPLUS 1,2.5-Thiadiarolidin-3-one, 2-{[(6-amino-2-benzoxazolyl)thio]methyl}-4,5-bis(phenylmethyl)-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-76-6 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4,5-bis(phenylmethyl)-2-{{(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 25 Aug 1999 ACCESSION NUMBER: 1999:529836 HCAPLUS

DOCUMENT NUMBER: 131:296959

A General Inhibitor Scaffold for Serine Proteases TITLE:

with

A General Inhibitor Scaffold for Serine Processes
a (Chymo)trypsin-Like Fold: Solution-Phase
Construction and Evaluation of the First Series of
Libraries of Mechanism-Based Inhibitors
Kuang, Rongre: Epp, Jeffrey B.; Ruan, Sumei; Yu,
Hongyi; Huang, Peng; He, Shu; Tu, Juan; Schechter,
Norman M.; Turbov, Jane; Froelich, Christopher J.;
Groutas, William C.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Journal of the American Chemical Society (1999),
121(35), 8128-8129
CODEN: JACAST; ISSN: 0002-7863
American Chemical Society
Journal

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: Journal

MENT TYPE: Journal UAGE: English The authors demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform embodies a general motif that renders the platform capable of binding to the active site of many serine proteases with a (chymo)trypsin-like fold in a predictable fashion and is amenable to the facile construction of libraries for lead identification and

facile constitues...

poptimization.

IT 170918-99-7P 170919-03-6P 189124-02-5P
247178-39-6P 247178-40-1P 247178-41-2P
RL: BAC (Biological activity or effector, except adverse); BSU

cogical
study, unclassified): SPN (Synthetic preparation): BIOL (Biological
study): PREP (Preparation)
(inhibitor: general inhibitor scaffold for serine proteases with a
(chymno)trypsin-like fold with solution-phase construction and

evaluation

uation of first series of libraries of mechanism-based inhibitors) 170918-99-7 HCAPLUS

170918-99-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylnethyl)-2-((phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry.

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylmethyl)-2-[(phenylsulfonyl)methyl]-4propyl-, 1,1-dioxide, (48)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-39-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobuty1)-5-(phenylmethy1)-2[(phenylsulfonyl)methy1]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 16 Mar 1999
ACCESSION NUMBER: 1999:172588 HCAPLUS
DOCUMENT NUMBER: 130:209985
TITLE: Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as serine protease inhibitors
Groutas, William C.; Kuang, Rongze
Wichita State University, USA
POT Int. Appl., 69 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent /
LANGUAGE: Epglish
FAMILY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

																	•			
		TENT				KIND DATE			APPLICATION NO.							DATE				
							-			-						-				
	WO	WO 9909977				A1 199			0304	. M	' WO 1998-US17406						19980821			
		W:	AU,	BR,	CA,	IS,	JP,	MX,	NZ											
		RW:	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,		
			PT,	SE																
	US	6420	401			B1		2002	0716	U	S 1	997-	9166	93		1	9970	822		
	AU	9890	298			А		1999	0316	A	U 1	998-	9029	В		1	9980	821		
	EP	1011	668			Al		2000	0628	E	P 1	998-	9421	92		1	9980	821		
		R:	DE,	GB																
PRI	ORIT	Y APP	LN.	INFO	.:					U	s I	997~	9166	93	1	A 1	9970	822		
																	0000	021		

OTHER SOURCE(S):

MARPAT 130:209985

AB Substituted 1,2,5-thiadiarolidin-3-one 1,1-dioxide deriva. I [R1, R3 = independently H, alkyl, aryl, aralkyl, alkaryl, substituted aryl; R2 = H, alkyl, aralkyl, alkyl, thydroxyalkyl, mino acid side chain; R4 = H, alkyl, aryl, aralkyl, mino acid side chain; P03R82, MCO, MHCHRTGOZRIO, MCORNI, aralkyl, aryl, aralkyl, aryl, aralkyl, aryl, aralkyl, aryl, mino acid side chain; R4 = H, alkyl, aryl, mino acid side chain; R4 = MCOZRIO, MCOZRIO, MCOZRIO, MCOZRIO, MCOZRIO, MCOZRIO, MCOZRIO, MCOZRIO, MCOZRIO, MCORNI, MCOZRIO, MCOZRIO, MCCOZRIO, MCCOZRIO, MCOZRIO, MCOZRIO,

ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN L4 (Continued)

247178-40-1 HCAPLUS

1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-5-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[([4S]-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) = G, H; m = 1-2; each R7 = amino acid side chain; each R8, R9 = alkyl, aryl, aralkyl, alkaryl, heterocyclyl; each R10-R15 = H, any group R8;

R16, R17 = heterocyclylalkyl; R18 = any group R8, NHR19; R19 = alkyl, aryl, aralkyl; with provisos], oligomers and combinatorial libraries contg. them, and methods of using them, are disclosed. Thus, title 1.

contg. them, and methods of using them, are disclosed. Thus, title d.

II showed apparent second-order rate consts. Kinact/KI (M-1s-1) of 119, 360, 27, 400, and 60 for inhibition of human leukocyte elastase, proteinase 3, and cathepsin G, resp. by in vitro assays. 220868-4-6pp, combinatorial library derivs. 220868-75-TDP, combinatorial library derivs. 220868-81-5pp, combinatorial library derivs. 220868-81-10P, combinatorial library derivs. 220868-86-91-DP, combinatorial library derivs. 220868-81-10P, combinatorial library derivs. 220868-81-10P, combinatorial library derivs. 220868-93-9DP, combinatorial library derivs. 220868-93-9DP, combinatorial library derivs. 220868-93-9DP, combinatorial library derivs. 220868-93-9P-020869-05-PP 220869-07-PP 220869-05-PP 220869-07-PP 2208

220869-41-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

gical tudy, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); IOL (Biological study); PREP (Preparation); USES (Uses) (preparation of amino acid-derived thiadiazolidinone dioxide derivs.

as serine protease inhibitors)
RN 220868-74-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(4-methoxyphenyl)methyl]-,
1,1-dioxide (9GI) (CA INDEX NAME)

RN 220868-75-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(3-phenoxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-80-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(acetyloxy)methyl}-5-{(4-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

220868-81-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(3-phenoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220868-92-8 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiarolidin-2-yl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-93-9 HCAPLUS
L-Phenylalanine, 4-chloro-N-[[[{1,1-dioxido-3-oxo-5-[{3-phenoxyphenyl)methyl}-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl]-

(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220868-86-0 HCAPLUS
Carbamic acid, [[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3-oxo-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

220868-87-1 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazoliddin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220868-98-4 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]aulfonyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220868-99-5 HCAPLUS L-Phenylalanine, 4-chloro-N-{{{[1,1-dioxido-3-oxo-5-{(3-phenoxyphenyl)methyl}-1,2,5-thiadiazolidin-2-yl}methyl}sulfonyl}methyl}-(SCI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-05-6 HCAPLUS
Carbamic acid, {[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}(phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

220869-06-7 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](phenylsulfonyl)-, phenylmethyl ester (9CI)(CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-16-9 HCAPLUS

Carbamic acid,
[2-[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-chiadiacolidin-2-yl]methyl](methylsulfonyl)amino]-2-oxoethyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] (methylsulfonyl)-, butyl ester [9CI] (CA INDEX

NAME)

RN 220869-14-7 HCAPLUS
CN Carbamic acid,
[2-[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-chiadiazolidin-2-yl]methyl](methylsulfonyl)amino}-2-oxoethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-26-1 HCAPLUS 1,2.5-Thiadiscolidin-3-one, 2-{(2-benzoxazolylthio)methyl}-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (901) (CA INDEX NAME)

RN 220869-27-2 HCAPLUS
CN 1.2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl,2-coxazoly1)thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(5-

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) phenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-30-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-2-{{3-phenyl-1,2,4-oxadiazol-5-yl}thio]methyl}-, 1,1-dioxide {9CI} (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-40-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[{(6-amino-2-benzoxazolyl)thio}methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-41-0 HCAPLUS 1.2.5-Thiadiarolidine-2-acetic acid, α -fluoro-3-oxo-4.5-bis[phenylmethyl]-, ethyl ester, 1,1-dioxide, (45)- (9CI) (CA INDEX

Absolute stereochemistry.

220869-64-7 220869-65-8 RL: RCT (Reactant) / RACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derive. IT

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-2-{[(5-phenyl-2-benzoxazolyl)thio]methyl]-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-39-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxdiazol-2-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-65-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

220869-61-4P 220869-62-5P 220869-63-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derivs.

serine protease inhibitors)

220859-61-4 HCAPLUS

1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5(phenylmethyl)-, 1,1-dimethylethyl ester, 1,1-dioxide, (45)- (9CI) (CA
INDEX NAME)

220869-62-5 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

(Continued) ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-63-6 HCAPLUS 1,2,5-Thiadiazolidine-2-acetamide, 4-(2-methylpropyl)-3-oxo-N-(2-phenylethyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 02 Oct 1998 ACCESSION NUMBER: 1998:622789 HCAPLUS

DOCUMENT NUMBER: 129:289796

TITLE:

AUTHOR (5):

129:289796
Kinetics of the hydrolysis of cyclic N-substituted sulfamides: 4-amino-2-cyclohexyl- and 4-amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5-thiadiazole 11,1-dioxides
Rozas, M. F.; Svartman, E. L.; Mirifico, M. V.; Vasini, E. J.
Instituto de Investigaciones Fisicoquimicas Te6ricas CORPORATE SOURCE:

Aplicadas (INIFTA), Facultad de Ciencias Exactas, Departamento de Quimica, Universidad Nacional de La Plata, La Plata, 1900, Argent. Journal of Physical Organic Chemistry (1998), 11(7), 489-494 SOURCE:

CODEN: JPOCEE; ISSN: 0894-3230 John Wiley & Sons Ltd.

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The hydrolysis reactions of 4-amino-2-phenethyl- and
4-amino-2-cyclohexyl2,3-dihydro-3-oxo-1,2,5-thiadiazole 1,1-dioxide (Ia and Ib) were
investigated at 24-73* in buffered aqueous solns. The observed rate
consts. (kobs) are independent of pH in the range ca 1-4 pH, but increase
with increase in pH above ca 4. A linear log kobs vs pH profile with

unit

slope is observed from pH ca 4 up to the highest exptl. pH (ca 10). The products are the corresponding new compds.: 2-amino-2-[(N-substituted-sulfamoyl)imino]acetic acid salts. The C=N bond of these compds. hydrolyzes further, in a slow reaction, to the sulfamide and oxalic acid derivs. The substrates decompose to the final products without accumulation

accumulation
of the acetic acid derivs. under these exptl. conditions. A mechanism is proposed. Rate consts. and activation parameters are given for the first reaction step. Owing to steric effects, the reaction rate is higher for the N-phenethyl-substituted derivative than for the 2-cyclohexyl-substituted derivative than for the 2-cyclohexyl-substituted derivative II 214216-09-8, 4-Amino-2-phenethyl-2,3-dihydro-3-oxo-1,2,5-thiadiazole 11,1-dioxide RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT

(Reactant); PROC (Process); RACT (Reactant or reagent)
(hydrolysis of cyclic N-substituted sulfamides)
214216-09-8 HCAPLUS
1,2,5-Thiadiazol-3-amine, 4,5-dihydro-5-(2-phenylethyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006.ACS on STN

ED Entered STN: 05 Aug 1998
ACCESSION NUMBER: 1998:487562 HCAPLUS
129:216561
Potent and specific inhibition of human leukocyte elastase, cathepsin G and proteinase 3 by sulfone derivatives employing the 1,2,5-thiadizablidin-3-one 1,1-doxide scaffold Grouts, William C.: Kuang, Rongze; Ruan, Sumei; Epp, Jeffrey B.: Venkateraman, Radhika; Truong, Tien M. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (1998), 6(6),

SOURCE: 661-671 CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd.

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: Journal English

This paper describes the results of structure-activity relationship studies in a series of heterocyclic mechanism-based inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold (I: R1 = iso-6b, benzyl: R2 = Bu, Me, benzyl: R2 (R2COCM64), etc.; L = So2Ph, SO2C6H4CL-4, etc.) and capable of interacting with the Sn and S'n subsites of a serine proteinase. Sulfone derivs. of I were found to be highly effective, time-dependent inhibitors of human leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3). The judicious selection of an R1 group (accommodated at the primary specificity site S1) that is based on the known substrate specificity of a target serine proteinase, was found to yield highly selective inhibitors. The primare of a benzyl group (R2 = benzyl) at the S2 subsite was found to lead to a pronounced enhancement

inhibitory potency. Furthermore, the effective use of computer graphics and modeling has led to the design of potent, water-soluble inhibitors.

results of these studies demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1-dioxide platform provides an effective means for appending

IT

212331-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylthio)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

212331-99-2 HCAPLUS
1,2,5-Thiadiscolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212332-00-8 HCAPLUS
Benzeneacetic acid, 3-[((35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylthio)methyl)-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-79-8P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

ogical study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREF (Preparation); RACT (Reactant or reagent) (preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3) 212331-79-8 HCAPLUS

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.
Double bond geometry as shown.

170919-03-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-77-6 HCAPLUS
Benzoic acid, 4-[[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-78-7 HCAPLUS
Benzoic acid, 4-[([35)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5-([phenylaulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzoic acid, 3-[([35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-[(phenylsulfonyl)methyl)-1,2,5-thiadiazolidin-2-yl]methyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 170918-99-7P 170919-01-4P 170919-03-6P
212331-77-6P 212331-78-7P 212331-80-1P
212331-81-2P 212331-82-3P 212331-83-4P
212331-82-5P 212331-97-0P
212331-97-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3)
RN 170918-99-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-1-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

N 170919-01-4 HCAPLUS N 1,2,5-Thiadiazolidin-3-one, -{phenylnechyl)-5-{(ZE)-3-phenyl-2-propenyl}-2-{(phenylsulfonyl)methyl}-, 1,1-dioxide, (45)- {9CI} (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

212331-80-1 HCAPLUS
Benzoic acid, 3-[([3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

212331-81-2 HCAPLUS
Benzoic acid, 2-[((3S)-3-{2-methylpropyl})-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl}methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-82-3 HCAPLUS Benzoic acid, 2-[[(3S)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5-

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN · (Continued) [(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 212331-83-4 HCAPLUS
CN Benteneacetic acid, 4-[[(3S)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl}- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[[(4-chlorophenyl)sulfonyl]methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-92-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenylpropyl)sulfonyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-94-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[[3-(trifluoromethyl)phenyl]sulfonyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-95-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(2-phenylethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) ((phenylsulfonyl)methyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-97-0 HCAPLUS
CN Benzeneacetic acid, 4-[[(3S)-1,1-dioxido-4-oxo-3-(phenylmethyl)-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMA'

10510026rtr L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 09 Apr 1998
ACCESSION NUMBER: 1998:200895 HCAPLUS
128:278642
Use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent inhibitors of serine proteinases
AUTHOR(S): Kung, Rongze; Venkataraman, Radhika; Ruan, Sumei;
Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, XS, 67260, USA
80(5), oloorganic & Medicinal Chemistry Letters (1998),

539-544
CODEN: BNCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The attachment of a phosphate leaving group to the
1,2,5-thiadiazolidin-3one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds was found
to yield highly potent, time-dependent inhibitors of human leukocyte
elastase (HLE).

17 205932-85-0P 205932-87-2P 205932-88-3P
205932-89-4P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPN (Synthatic preparation) logical
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and
isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent
inhibitors of serine proteinases)
205932-85-0 HCAPLUS
Phosphoric acid, dimethyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX
NAME) 205932-87-2 HCAPLUS
Phosphoric acid, dibutyl (4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX

L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 30 Aug 1997 ACCESSION NUMBER: 1997:555602 HCAPLUS DOCUMENT NUMBER: 127:257045 Competitive particle concentration fluorescence immunoassays for measuring antidiabetic drug levels mouse plasma Bright, Stuart W.; Tinsley, Frank C.; Dominianni, Samuel J.; Schmiegel, Klaus K.; Fitch, Lora L.; Gold, AUTHOR (5): Gerald Gerau Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA Journal of Immunological Methods (1997), 207(1), CORPORATE SOURCE: CODEN: JIMMBG; ISSN: 0022-1759 COURN: JIRMSG; ISSN: 0022-1759

R: Elsevier
TYPE: Journal:
: English
competitive particle concentration fluorescence immunoassays were PUBLISHER: DOCUMENT TYPE: LANGUAGE:

developed
to measure blood levels of analogs of antidiabetic drugs being tested in diabetic mice. Ligands that contained the active pharmacophores were conjugated to PPD for immunization and to β-phycoerythrin for use as a tracer in the immunoassays. Approx. 90% of 262 compds. assayed were detectable at less than 120 nM in plasma which was well below the estimated therapeutic level of 1 μM for lowering blood glucose. These data were used to define the bioavailability of test compds. and assist in decisions

of constructing active analogs. Of addnl. interest, we noted crossreactivity of one monoclonal antibody for 3 different compound classes

that are all known to bind with varying affinities to peroxisome proliferator-activated receptors.
196079-43-3
RE: ANT (Analyte); ANST (Analytical study)
(competitive particle concentration fluorescence immunoassays for

(competitive percents)
suring
antidiabetic drug levels in mouse plasma)
196079-43-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[2-(2-phenyl-4-oxazolyl)ethoxy]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR 13

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

205932-88-3 HCAPLUS
Phosphoric acid, [4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl bis(phenylmethyl) ester (9CI) (CA INDE: NAME)

205932-89-4 HCAPLUS
Phosphoric acid, [4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5-thiadiazolidin-2-yl]methyl diphenyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

FORMAT

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued)

L4 ANSWER JO OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 09 Apr 1997
ACCESSION NUMBER: 1997:226643 HCAPLUS
DOCUMENT NUMBER: 126:287581
TITLE: Structure-Based Design of a General Class of Mechanism-Based Inhibitors of the Serine Proteinases Employing a Novel Amino Acid-Derived Heterocyclic Scaffold
AUTHOR(S): Groutas, William C.; Kuang, Rongre; Venkataraman, Radhika: Epp, Jeffrey B.; Ruan, Sumei: Prakash, Om Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
SOURCE: Biochemistry (1997), 36(16), 4739-4750
CODEN: BICHAW: ISSN: 0006-2960
American Chemical Society
Journal

PUBLISHER: DOCUMENT TYPE:

JAGE: English We describe in this paper the structure-based design of a general class

heterocyclic mechanism-based inhibitors of the serine proteinases that embody in their structure a novel peptidominetic scaffold (1,2,5-thiadiazolidin-3-one 1,1-dioxide). Sulfone derivs. of this class were time-dependent, potent, and highly efficient irreversible inhibitors of human leukocyte elastase, cathepsin G, and proteinase 3. The

partition $% \left(1\right) =\left(1\right) \left(1\right) +\left(1\right) \left(1\right) \left(1\right) +\left(1\right) \left(1\right)$

and 1. We furthermore demonstrate that these inhibitors exhibit remarkable ${\cal C}$

selectivity that is dictated by the nature of the Pl residue and is consistent with the known substrate specificity reported for these enzymes. Thus, inhibitors with small hydrophobic side chains were effective inhibitors of elastase, those with aromatic side chains of cathepsin G, and those with a basic side chain of bovine trypsin. Taken together, the findings cited herein reveal the emergence of a general class of stable mechanism-based inhibitors of the serine proteinases

can be readily synthesized using amino acid precursors. Biochem. and high-field NMR studies show that the interaction of this class of inhibitors with a serine proteinase results in the formation of a stable acyl complex(es) and the release of benzenesulfinate, formaldehyde, and a low mol. weight heterocycle. The data are consistent with initial

formation of a Michaelis-Menten complex, acylation of Ser195, and tandem loss of

or a michaelis-Menten complex, acylation of Ser195, and tandem loss of leaving group. The initial HLE-inhibitor complex reacts with water generating formaldehyde and a stable HLE-inhibitor complex. Whether the initial HLE-inhibitor complex also reacts with His57 to form a third complex is not known at this point. The desirable salient parameters associated with this class of inhibitors, including the expeditious generation of structurally diverse libraries of inhibitors based on I, suggest that this class of mechanism-based inhibitors is of general applicability and can be used in the development of inhibitors of human and viral serine proteinases of clin. relevance.
170918-99-79 170919-03-69 189124-00-39 189124-05-99 RL: BAC (Biological activity or effector, except adverse); BSU logical study, unclassified); SPN (Synthetic preparation); BIOL (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and structure activity relations of mechanism-based inhibitors

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) of human leukocyte serine proteinases employing a novel amino acid-derived heterocyclic scaffold) 170918-99-7 KCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

170919-03-6 KCAPLUS
1,2,5-Thiadiasolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylmilfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-00-3 HCAPLUS 1,2,5-Thiadizolidin-3-one, 4-ethyl-5-(phenylmethyl)-2-[(phenylaulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) [(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylmethyl)-2-(phenylmulfonyl)methyl]-4propyl-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-04-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{1-methylethyl}-5-(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

189124-06-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-butyl-5-(phenylmethyl)-2-

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 01 Dec 1995
ACCESSION NUMBER: 1995:954574 HCAPLUS
COCUMENT NUMBER: 123:340140
Novel serine protease inhibitors: derivatives of isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide

INVENTOR(s): Groutas, William C.
Wichita State University, USA
PCT Int. Appl., 93 pp.
CODEM: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE		APPLICATION NO.						DATE			
WO									WO 1995-US236									
	W:	AM,																
		GE.	HU,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LK,	LT,	LU,	LV,	MD,	MG,	MN,	MW,	
		NL.	NO.	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SI,	SK,	TJ,	TT,	UA,	υz,	VN	
	RW:	AT.	BE.	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SÉ	
US	5550	139			A		1996	0827		US 1	994~	1773	52		1	9940	103	
CA	2175	913			A1		1995	0713		CA 1	995~	2179	913		1	9950	103	
AU	951	998			A		1995	0801		AU 1	995-	1599	В		1	9950	103	
AU	686	116			B2		1998	0205										
EP	739	338			A1		1996	1030		EP 1	995-	9080	03		1	9950	103	
EP	739	338			B1		2002	0410										
	R:	AT,	BE,	ÇH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	ΙT,	LI,	LU,	MC,	NL,	PT,	
SE																		
JP	0950	9922			T		1997	1007										
AT	215	38			T		2002	0415			995-							
NZ	329	766			A		2001	0223		NZ 1	998-	3297	66		1	9980	216	
PRIORIT	Y AP	PLN.	INFO	.:						US 1	994-	1773	52		A 1	9940	103	
										WO 1	995~	11523	6		w 1	9950	103	

OTHER SOURCE(S): MARPAT 123:340140

Various isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide derivs., e.g. I $\{X=CR2, \{un\}$ substituted NH; RI = H, alkyl, $\{un\}$ substituted benzyl, indolylalkyl, etc.; Y= non-steroidal antiinflammatory residue, H, protected amino acid, acyloxy, etc.], and their use to reduce or inhibit the activity of serine proteases, are claimed. The compost are useful as anti-inflammatory and anti-metastatic agents. For example, 4-benzylisothiazolidin-3-one 1,1-dioxide underwent

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
N-alkylation with ClCH2SPh and Et3N in MeCN, followed by S-oxidn. with
m-ClC6H4(O)OOH in CH2Cl2 (904), to give title compd. II. In an in vitro
assay, II had an apparent 2nd-order inactivation rate const. (kobs/[I]

M-1
s-1) of 960 against cathepsin G. A variety of compds. were prepd, and/or tested against cathepsin G, human leukocyte elastase, and/or proteinase-3.
If 170919-16-1P
RL: RCT (Reactant), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-16-1 RCAPLUS
CN 12,25-thiadiazolidin-3-one, 4-(phenylmethyl)-5-(3-phenyl-2-propenyl)-2-((phenylthio)methyl)-, 1,1-dioxide, (S-(E))- (SCI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 170919-15-0P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-15-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4,5-bis(phenylmethyl)-2-[(phenylthio)methyl]-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 170919-03-6 170919-21-8 170919-22-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); THU (Therapeutic use); BIOL (Biological study);

USES (Uses)

{Uses} (Uses) (preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)
RN 170919-03-6 HCAPLUS
CN 1,2.5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-21-8 HCAPLUS 1/03/5-71-0 mcArbus 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[(phenylsulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 170919-22-9 HCAPLUS

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

153044-45-2P 170918-99-7P 170919-01-4P

Absolute stereochemistry.

170918-99-7 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4,5-bis(phenylmethyl)-2(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-((25)-3-phenyl-2-propenyl)-2-((phenylsulfonyl)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1.2.5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:124451 HCAPLUS
DOCUMENT NUMBER: 120:124451 SUbstituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides:
a new class of potential mechanism-based inhibitors

AUTHOR (S):

human leukocyte elastase and cathepsin G
Groutas, William C.; Kuang, Rongze; Venkataraman,
Radhika
Dep. Chem., Wichita State Univ., Wichita, KS, 67260,
USA
Biochemical and Biophysical Research Communications
(1994), 198(1), 341-9
CODEN: BBRCA9; ISSN: 0006-291X
Journal
English

CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: GI

A series of substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides (I, R = benzyl; Rl = H, Me, benzyl, CH2CO2-tert-Bu or CH2CO2-benzyl) was prepd, and their in vitro inhibitory activity toward human leukocyte elastase

cathepsin G was investigated. These compds. inactivated the 2 enzymes efficiently and in a time-dependent fashion.
153044-45-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and human leukocyte elastase and cathepsin G

inhibition by)
RN 153044-45-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Jan 1991 ACCESSION NUMBER: 1991:23940 HCAPLUS

DOCUMENT NUMBER: TITLE:

114:23940

AUTHOR(S): CORPORATE SOURCE:

Intra- and intermolecular α-sulfamidoalkylation reactions Lee, Chai Ho; Kohn, Harold Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA USA JOURNAL of Organic Chemistry (1990), 55(25), 6098-104 CODEN: JOCEAH: ISSN: 0022-3263 JOURNAL

SOURCE:

DOCUMENT TYPE:

English CASREACT 114:23940

LANGUAGE: OTHER SOURCE(S): GI

The utility of $\alpha\text{-sulfamidoalkylation}$ processes for the generation of sulfamidea has been examined. Both intra- and intermol. a sulfamioalkylation transformations were observed to proceed in moderate

good yields. The generality of these processes has been demonstrated using N,N'-di(aryl-substituted) sulfamides, and the utility of these reactions was examined for the preparation of cyclic sulfamides of novel structure. Thus, reaction of PhCHRIMISORINE with ECOZCH(OEL)2 in the presence of CF3COZH gave 74% dithiatetrazocinedicarboxylate tetraoxide I, whereas reaction of 3-MeOCSH(ACK)MSOZNHZ with ECOZCH(OEL)2 in CF3COZH followed by methylation gave benzothiadiarepinecarboxylate dioxide II. The crystal structures of I and II were determined 130670-00-7P

באיסיטיייטייין RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Reactant or reagent)
(preparation and cyclization of)
130670-00-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-hydroxy-5-(2-phenylethyl)-, 1,1-dioxide,
monosodium salt (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

• Na

=> log y COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.69	340.84
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-24.75	-24.75

STN INTERNATIONAL LOGOFF AT 14:04:52 ON 21 DEC 2006

Connecting via Winsock to STN

```
Welcome to STN International! Enter x:x
```

LOGINID: SSPTANAG1626

PASSWORD:

NEWS LOGIN

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
      2
NEWS
      3
         AUG 09
                 INSPEC enhanced with 1898-1968 archive
NEWS
                 ADISCTI Reloaded and Enhanced
NEWS
         AUG 28
                CA(SM)/CAplus(SM) Austrian patent law changes
         AUG 30
NEWS
                 CA/CAplus enhanced with more pre-1907 records
         SEP 11
NEWS
      6
         SEP 21
                 CA/CAplus fields enhanced with simultaneous left and right
NEWS
                 truncation
         SEP 25
                 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS
     8
                 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS
     9
         SEP 25
                 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
         SEP 25
NEWS 10
                 CEABA-VTB classification code fields reloaded with new
         SEP 28
NEWS 11
                 classification scheme
                 LOGOFF HOLD duration extended to 120 minutes
         OCT 19
NEWS 12
NEWS 13
         OCT 19
                 E-mail format enhanced
                 Option to turn off MARPAT highlighting enhancements available
         OCT 23
NEWS 14
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 15
         OCT 23
                 multiple databases
                 The Derwent World Patents Index suite of databases on STN
         OCT 23
NEWS 16
                 has been enhanced and reloaded
                 CHEMLIST enhanced with new search and display field
NEWS 17
         OCT 30
                 JAPIO enhanced with IPC 8 features and functionality
         NOV 03
NEWS 18
                 CA/CAplus F-Term thesaurus enhanced
         NOV 10
NEWS 19
                 STN Express with Discover! free maintenance release Version
NEWS 20
         NOV 10
                 8.01c now available
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 21
         NOV 20
                 additional databases
                 CA/CAplus to MARPAT accession number crossover limit increased
NEWS 22
         NOV 20
                 to 50,000
NEWS 23
         DEC 01
                 CAS REGISTRY updated with new ambiguity codes
                 CAS REGISTRY chemical nomenclature enhanced
NEWS 24
         DEC 11
         DEC 14
NEWS 25
                 WPIDS/WPINDEX/WPIX manual codes updated
                 GBFULL and FRFULL enhanced with IPC 8 features and
NEWS 26
         DEC 14
                 functionality
                 CA/CAplus pre-1967 chemical substance index entries enhanced
NEWS 27
         DEC 18
                 with preparation role
                 CA/CAplus patent kind codes updated
NEWS 28
         DEC 18
                 MARPAT to CA/CAplus accession number crossover limit increased
NEWS 29
         DEC 18
                 to 50,000
                 MEDLINE updated in preparation for 2007 reload
NEWS 30
         DEC 18
              NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
NEWS EXPRESS
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
              STN Operating Hours Plus Help Desk Availability
NEWS HOURS
```

Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8 NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 12:18:58 ON 21 DEC 2006

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 12:19:08 ON 21 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0 DICTIONARY FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

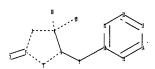
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10510026RTR.str



```
chain nodes :
7  9  18  19
ring nodes :
1  2  3  4  5  10  11  12  13  14  15
chain bonds :
2-7  4-18  4-19  5-9  9-10
ring bonds :
1-2  1-5  2-3  3-4  4-5  10-11  10-15  11-12  12-13  13-14  14-15
exact/norm bonds :
1-2  1-5  2-3  2-7  3-4  4-5  4-18  4-19  5-9
exact bonds :
9-10
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15
```

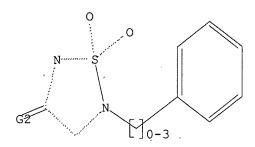
G1:H,CH3

G2:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Me G2 O, S

Structure attributes must be viewed using STN Express query preparation.

=> s 11 SAMPLE SEARCH INITIATED 12:19:35 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 62 TO ITERATE

100.0% PROCESSED 62 ITERATIONS 50 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 768 TO 171

PROJECTED ITERATIONS: 768 TO 1712 PROJECTED ANSWERS: 576 TO 1424

L2 50 SEA SSS SAM L1

=> s 11 full FULL SEARCH INITIATED 12:19:40 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1006 TO ITERATE

100.0% PROCESSED 1006 ITERATIONS 770 ANSWERS

SEARCH TIME: 00.00.01

L3 770 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'HCAPLUS' ENTERED AT 12:19:44 ON 21 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Dec 2006 VOL 145 ISS 26 FILE LAST UPDATED: 20 Dec 2006 (20061220/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 33 L3

 \Rightarrow d ed ibib abs hitstr 1-33

145:211037
Preparation of pyrazolyl aryl ureas as modulators of the protein kinase activation state for treatment of inflammation and hyperproliferative diseases Flynn, Daniel L.; Petillo, Peter A. Deciphera Pharmaceuticals, LLC, USA PCT Int. Appl., 305pp. CODEN: PIXXD2
Patent English 2
2

INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT:

PATE	ENT I	NFOR	MATI	ON:															
	PAT	ENT	NO.			KIN	D	DATE		i	APPL	ICAT	ION	NO.		DATE			
							-												
	WO	2006	0810	34		A2	•	2006	0803	1	NO 2	005-	US47	597		2	0051	223	
	WO	2006	0810	34		A3		2006	1123										
		w:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
			CN,	co.	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
			GE.	GH.	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ĸм,	KN,	Κ₽,	KR,	
			KZ.	LC.	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	ΜK,	MN,	MW,	MX,	
			MZ.	NA.	NG.	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	ΡŤ,	RO,	RU,	SC,	SD,	SE,	
			SG,	sĸ,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	ΤZ,	UA,	UG,	US,	UΖ,	VC,	
				YU,															
		RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ΒJ,	
			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,	GH,	
			GM,	KE,	LS,	MW,	M2,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	zw,	AM,	ΑZ,	BY,	
			KG,	ΚZ,	MD,	RU,	TJ,	TM											
PRIC	DRITY	APP	LN.	INFO	.:					1	US 2	004-	6389	87P		₽ 2	0041	223	

MARPAT 145:211037

OTHER SOURCE(S):

Novel compds. and methods of using those compds. for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and diseases

characterized by hypervascularization are provided. In a preferred

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

PAGE 1-A

903567-40-8 HCAPLUS Urea, $N-\{3-\{1,1-\text{dimethy}\}=1-\{3-\{\{1,1-\text{dioxido}-3,4-\text{dioxo}-1,2,5-\text{thiadiazolidin}-2-y\}\}$ methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(SCI) (CA INDEX NAME)

embodiment, the compds. of the invention modulate the activation state of p38 kinase protein, abl kinase protein, bcr-abl kinase protein, braf kinase protein, VEGFR kinase protein, cpr-abl kinase protein, braf compds. of the invention I have general formula (RI-(XI))m-A-NN-L-NN-C[E]q-(Y)t-Q wherein RI = aryl, heteroaryl, and heterocylyl; X and Y = individually O, S, alkynyl, alkenyl, etc.; A = an arom., monocyloheterocyclic or bicycloheterocyclic ring; D = Ph or a 5-6-membered heterocyclic ring; E = Ph, pyridinyl, or pyrimidinyl; L = -C(O) - or -S(O)2-; j,m,qt = O-1; and Q = a substituted ring or ring system. Over 500 compds. were prepd. For example, hydrogenation of 3-(3-aminophenyl) acrylic acid Me ester provided the propionate, which was subsequently converted to the hydrazine. Reaction of the hydrazine with 4.4-dimethyl-3-coxpentanenitrile afforded Me
3-[3-(3-tert-butyl-5-amino-IN-pyrazole-1-yl)phenyl|propionate. which was coupled with 1-naphthyl isocyanate and reduced to provide urea II. In a competition assay with SKF 86002 as a fluorescent probe, II inhibited p38 MAP kinase with ICSO of

of

45 nM.
697369-58-3P 903567-40-8P
RL: DNA (Drug mechanism of action); PAC (Pharmacological activity); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrazolyl aryl ureas as modulators of
protein kinase activation state for treating inflammation and
proliferative disorders)
897369-58-3 HCAPLUS
Ulrea. ΙT

RN 897369-58-3 HCAPLUS
CN Urea,
N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-3,4-dioxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-IH-pyrazol-5-yl)- (9CI)
(CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-35-2P, 1-[5-tert-Butyl-2-[3-[[(S)-3-methyl-1,1,4-trioxo-

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-{[(R)-3-methyl-1, 1, 4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-{[(1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-3-yl]-2-naphthalenecarboxamide 872171-62-5P, 1-[5-tert-Butyl-2-[3-

{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-63-6P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methyl]phenyl]-2H-pyrazol-3-y1]-3-(4-chlorophenyl)urea 872171-73-8P, 1-[5-tert-Butyl-2-[3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-methoxynephthalen-1-yl)urea
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USes)

(Uses)

(JS8 kinase inhibitor; preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases)

RN 872171-35-2 HCAPLUS

CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-{{(3S)-3-methyl-1,1-dioxido-4-oxo-1,2,5-chiadiarolidin-2-yl]methyllphenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-37-4 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-{3-([(3R)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thidiazolidin-2-yl]methyl]phenyl|-1H-pyrazol-5-yl|-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-57-8 HCAPLUS 2-Naphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9C1) (CA INDEX NAME)

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-62-5 HCAPLUS
Urea, N-{3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(SCI) (CA INDEX NAME)

o/21/1-03-0 MCAPLUS
Urea, N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME) 872171-63-6 HCAPLUS

(Continued)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

IT 872171-36-3P, 1-[5-tert-Butyl-2-(3-{[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-39-6P, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl-2-[3-[5-(4-methoxybenzyl-2-[3-[5-(4-methoxybenzyl-2-[3-[3-(4-methoxybenzyl-2-[3-[3-(4-methoxybenzyl-2-[3-[3-(4-methoxybenzyl-2-[3-[3-(4-methoxybenzyl-2-[3-[3-(4-methoxybenzyl-2-[3-(1,2,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of pyrazolyl aryl ureas as modulators of protein kinase activation state for treatment of inflammation and hyperproliferative diseases) RN 872171-36-3 HCAPLUS CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(3R)-5-[(4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Urea, N-(3-(1,1-dimethylethyl)-1-(3-[(5-[(4-methoxyphenyl)methyl)-1,1-

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-lH-pyrazol-5-yl]-N'-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

872171-49-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}-1H-pyrazol-5-yl]-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 28 Jul 2006 ACCESSION NUMBER: 2006:739358 HCAPLUS DOCUMENT NUMBER: 145:377543

TITLE:

145:377543
Isothiazolidinone heterocycles as inhibitors of protein tyrosine phosphatases: Synthesis and structure-activity relationships of a peptide

Yue, Eddy W.; Wayland, Brian; Douty, Brent; Crawley, Matthew L.; McLaughlin, Erin; Takvorian, Amy; Wasserman, Zelda; Bower, Michael J.; Wei, Min; Li, Yanlong; Ale, Paul J.; Gonneville, Lucie; Wynn, Richard; Burn, Timothy C.; Liu, Phillip C. C.; Combs, Andrew P.

Richard' Burn, Timothy C.: Liu, Phillip C. C. Co Andrew P. Discovery Chemistry, Experimental Station, Incyte Corporation, Wilmington, DE, 19880, USA Bioorganic & Medicinal Chemistry (2006), 14(17), 5833-5849 CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier B.V.

PUBLISHER: DOCUMENT TYPE:

English

LANGUAGE:

scaffold

Oxo- and trioxo-substituted isothiazolidinylphenylalanines are prepared

tyrosine mimetics by Suzuki coupling reactions of chloroisothiazolidinones and chlorodioxoisothiazolidinones with N-Boc-4-borono-L-phenylalanine derivs.: the isothiazolidinylphenylalanines (with or without subsequent hydrogenation) are incorporated into dipeptides prepared as human protein tyrosine phosphatase 18 (PTP18) inhibitors such as I. Of the compds. tested, I is the most potent inhibitor of PTP18 with an IC50 value of 40 nM; the corresponding mixture of isothiazolidinone disatereomers inhibits PTP18 with an IC50 value of 80 nM, and the separated (R)-isothiazolidinone disatereomer inhibits PTB18 with an IC50 value of 15.5 µM; the related dispeptides prepared inhibit PTP18 less potently than either I or the mixture

mixture of isothiazolidine diastereomers containing I. Crystal structures of dioxothiazolidinone-substituted dipeptide and a dioxoisothiazolinone-substituted dipeptide bound to PTP1B are determined by X-ray

crystallog.; the low energy conformation found by ab initio calcas, for the saturated

L4 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) heterocycle more closely approaches the conformation obtained upon

binding
to PTPLB than that of the unsatd, heterocycle.

IT 850315-22-99
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of isothiazolone- and dioxoisothiazolone-substituted phenylalanine-containing dipeptide amides and their activities as

n PTP1B inhibitors) 850315-22-9 HCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-20-7P 850315-21-8P 850315-23-0P 910606-95-0P 910606-97-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of isothiszolone- and dioxoisothiazolone-substituted phenylalenine-containing dipeptide amides and their activities as

n
PTP1B inhibitors;

850315-20-7 HCAPLUS

Carbamic acid, {(IS)-1-[[4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiarolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,

1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-21-0 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

850315-23-0 HCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 910606-97-2 HCAPLUS
CN L-Phenylalaninamide,
L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]-N-pentyl-, mono(trifluoroacetate) (9CI) {CA
INDEX NAME)

CM. 1

CRN 910606-96-1 CMF C32 H39 N5 O5 S

Absolute stereochemistry.

CM 2

CRN . 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: THIS

THERE ARE 39 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

910606-95-0 HCAPLUS Benzenepropanamide, α-amino-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2.5-thiadiazolidin-2-yl]-N-pentyl-, (αS)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 910606-94-9 CMF C23 H30 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

L4 ANSMER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN
ED Entered STN: 07 Jul 2006
ACCESSION NUMBER: 2006:655575 HCAPLUS
DOCUMENT NUMBER: 145:124558
ITILE: modulators
INVENTOR(S): Flynn, Daniel L.; Petillo, Peter A.
Deciphera Pharmaceuticals, LLC, USA
PCT Int. Appl., 974 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.													ATE	
			-											
WO 20060719	40	A2		2006	0706	,	WO 2	005-	US47	270		2	0051	223
	AG, AL,													
CN,	CO, CR,	CU.	CZ.	DE.	DK.	DM.	DZ.	EC.	EE.	EG.	ES.	FI.	GB,	GD,
	GH, GM,													
	LC, LK,													
	NA, NG,													
56	SK, SL,	SM.	SY.	TJ.	TM.	TN.	TR.	TT.	TZ.	UA,	UG,	US,	UZ,	VC,
	YU, ZA,			,										
	BE, BG,			CZ.	DE.	DK.	EE.	ES.	FI.	FR.	GB,	GR,	HU,	IE,
	IT, LT,	LU.	LV.	MC.	NL.	PL.	PT.	RO.	SE.	SI.	SK,	TR,	BF,	BJ,
	CG, CI,													
GM.	KE, LS,	MW.	MZ.	NA.	SD,	SL.	52,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
	KZ, MD,													
PRIORITY APPLN.							US 2	004-	6389	68 P		P 2	0041	223

							US 2	004-	6389	86P		P 2	0041	223
•							US 2	004-	6389	87P		P 2	0041	223

US 2004-639087P

P 20041223

OTHER SOURCE(S):

MARPAT 145:124558

The invention relates to title compds. I [A2 = bicyclic fused aryl, bicyclic fused heteroaryl, and bicyclic fused heteroaryl, etc.: Al = pyrazolyl, Ph, pyridyl, pyrimidinyl, etc.: W, Y = CRM4, NR3 or O (wherein W and Y are not simultaneously O): X = O, S or NR3: D = Ph, heteroaryl,

ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) heterocycly1, etc.; R3 = H, alky1, cycloalky1, Ph; R4 = H, alky1, hydroxyalky1, etc.) which are useful for the treatment of inflammatory conditions, hyperproliferative diseases, cancer, and diseases characterized by hypervascularization. Over 500 compds. I were prepd. E.g., a multi-step synthesis of II, starting from m-aminobenzoic acid,

given. Compds. I were tested against various kinases (ICSO values were given for representative compds. I). In a preferred embodiment, modulation of the activation state of p36 kinase protein c-Abl kinase protein, Bcr-Abl kinase protein, B-raf kinase protein, vEGFR kinase protein, or PDGFR kinase protein comprises the step of contacting said kinase protein with the novel compds. I. 897369-58-3P 897369-62-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea)

(Uses)

(preparation of pyrazolyl Ph ureas as enzyme modulators for treating

cancer
 and hyperproliferative diseases)
RN 897369-58-3 HCAPLUS
CN Urea.
N-(4-chlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-3,4-dioxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-IH-pyrazol-5-yl]- (9CI)
(CA INDEX NAME)

PAGE 1-A

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) PAGE 2-A

RN 897369-62-9 HCAPLUS ,
CN Urea,
(-2, 3-dichlorophenyl)-N'-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-3,4-dioxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl}-

(CA INDEX NAME)

PAGE 1-A

L4 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 29 Dec 2005

ACCESSION NUMBER: 2005:1346235 HCAPLUS

DOCUMENT NUMBER: 144:88279

TITLE: Preparation of 1-pyrazoly1-3-phenylurea p38 MAP

kinase

inhibitors as antiinflammatory medicaments Flynn, Daniel L.; Petillo, Peter A. USA U.S. Pat. Appl. Publ., 214 pp., Cont.-in-part of U.S. Ser. No. 746,460. CODEN: USXXCO INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

			APPLICATION NO.	
			US 2004-886329	
US 2004180906	A1	20040916	US 2003-746460	20031224
		20061205		
			WO 2005-US23100	20050630
WO 2006014290	A3	20060427		
			BA, BB, BG, BR, BW, B	
			DM, DZ, EC, EE, EG, E.	
			IN, IS, JP, KE, KG, KI	
			MA, MD, MG, MK, MN, M	
			PL, PT, RO, RU, SC, S	
	TJ, TM,	TN, TR,	TT, TZ, UA, UG, US, U	Z, VC, VN, YU,
ZA, ZM, ZW				
			DK, EE, ES, FI, FR, G	
15, IT, LT,	LU, MC,	NL, PL,	PT, RO, SE, SI, SK, T ML, MR, NE, SN, TD, T	K, BI, BJ, CI,
CG, CI, CM,	GA, GN,	GO, GW,	SZ, TZ, UG, ZM, ZW, A	M NO RV KG
KZ, MD, RU,		30, 31,	52, 12, 00, EM, EW, A	M, ME, DI, NO,
PRIORITY APPLN, INFO.:			us 2003-746460	A2 20031224
PRIORITI AFFEN. INTO			05 2005 110100	, L
			US 2002-437304P	P 20021231
			US 2002-437403P	P 20021231
•			US 2002-437415P	P 20021231
			US 2002-437487P	P 20021231
			-	
			US 2003-463804P	P 20030418
			US 2004+886329	A 20040706

OTHER SOURCE(S): MARPAT 144:88279

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Title compds. (R1Xj)mA(NH)pLn(NH)pDEqYtQ [I; wherein Rl = (un)substituted (hetero)aryl; X, Y = independently O, S, NR6, NR6SO2, NR6CO, alkynyl, alkenyl, alkylene, O(CH2)h, NR6(CH2)h, wherein for each alkylene,

O(CH2)h, and NR6(CH2)h, one of the methylene groups may be substituted with CO; h

1-4; A = (un)substituted aryl, hetero(bi)cyclyl; D = (un)substituted Ph, pyrazolyl, pyrrolyl, imidazolyl, oxazolyl, thiazolyl, furyl, pyridyl, pyrimidyl; E = (un)substituted Ph, pyridinyl, pyrimidinyl; L = CO, 502;

j, m, n, p, q, t = independently 0, 1; Q = (un)substituted heterocyclyl, Ph, etc.; R6 = independently H, alkyl, allyl, TMS(CH2)2; with exceptions]

prepared as p30 MAP kinase inhibitors. In a preferred embodiment, modulation of the activation state of p30 kinase protein comprises the step of contacting the α -C helix, the α -D helix, the catalytic loop, the switch control ligand sequence, or the C-lobe residues of the kinase protein with I (no data). Although the methods of preparation

not claimed, prepns. and/or characterization data for .apprx.150 examples of 1

and many intermediates are included. For example, hydrogenation of 3-(3-aminophenyl)acrylic acid Me ester using 10% Pd/C in EtOH provided

propionate, which was treated with NaNO2 in the presence of 6N HCl and SnCl2*2H2O to give the hydrazine. Reaction of the hydrazine with 4,4-dimethyl-3-oxopentanenitrile in EtOH and 6N HCl afforded Me 1-(3-(3-tert-butyl-5-amino-lH-pyrazole-1-yl)phenyl)propionate. Coupling of the amine with 1-naphthyl isocyanate in CH2Cl2, followed by reduction

with LioH in THF/MeOH/H2O provided the urea II. In a competition assay with SKF 66002 as a fluorescent probe, the latter inhibited p38 MAP kinase

with IC50 of 45 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a wide variety of inflammatory conditions (no data). 872171-35-2P, 1-[5-tert-Buty1-2-[3-[{(5)-3-methyl-1,1,4-trioxo-

[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-37-4P, 1-[5-tert-Butyl-2-[3-[[(R)-3-methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl)urea 872171-57-8P, N-[3-tert-Butyl-1-[3-[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]-2-

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) naphthalenecarboxamide 872171-62-5P, 1-{5-tert-Butyl-2-{3-

[(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methy1]pheny1]-2H-pyrazol-3-y1]-3-(naphthalen-1-y1)urea 872171-63-6P, 1-[5-tert-Buty1-2-[3-

 $\{(1,1,4-trioxo-[1,2,5]thiadiazolidin-2-y1)methy1]pheny1\}-2H-pyrazol-3-y1\}-3-(4-chloropheny1)urea 072171-73-0P, 1-[5-tert-Buty1-2-[3-$

[(1.1,4-trioxo-[1,2,5]thiadia2olidin-2-yl)methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-methoxynaphthalen-1-yllurea RL: PAC (Pharmacological activity), SPN (Synthetic preparation); THU (Therapeutic use); SIOL (Biological study); PREP (Preparation); USES

(Uses)
(D38 kinase inhibitor; prepn. of (pyrazolyl)(phenyl)urea p38 kinase inhibitors as antiinflammatory agents)
872171-35-2 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[{(3S)-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

872171-37-4 HCAPLUS Urea, N- $\{3-\{1,4\}$ HCAPLUS Urea, N- $\{3-\{1,4\}$ HCAPLUS HT41, 1-dioxido-4-oxo-1,2,5-thidiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

872171-57-8 HCAPLUS
2-Naphthalenecarboxamide, N-[3-(1,1-dimethylethyl)-1-[3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-IM-pyrazol-5-yl]- (9CI) (CA

872171-62-5 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl-(9CI) (CA INDEX NAME)

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

872171-63-6 HCAPLUS
Urea, N-{4-chlorophenyl}-N'-{3-(1,1-dimethylethyl)-1-{3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

872171-73-8 HCAPLUS
Urea, N-[3-(1,1-dimethylethyl)-1-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-lH-pyrazol-5-yl]-N'-(4-methoxy-1-naphthalenyl)- (9CI) (CA INDEX NAME)

IT 872171-36-3P, 1-[5-tert-Butyl-2-[3-[[5-(4-methoxybenzyl)-(R)-3-

methyl-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(naphthalen-1-yl]vrea 872171-39-69, 1-[5-tert-Butyl-2-[3-[5-(4-methoxybenzyl]-1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea 872171-49-89, 1-[5-tert-Butyl-2-[3-([1,1,4-trioxo-[1,2,5]thiadiazolidin-2-yl]methyl]phenyl]-2H-pyrazol-3-yl]-3-(4-fluorophenyl)urea RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of (pyrazolyl) (phenyl)urea p38 kinase inhibitors as antinflammatory agents) 872171-36-3 HCAPLUS CN Urea, N-[3-(1,1-dimethylethyl)-1-[3-[([3R)-5-[(4-methoxyphenyl)methyl]-3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-1-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

L4 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

872171-39-6 HCAPLUS Urea, N-{3-(1,1-dimethylethyl)-1-[3-[{5-[(4-methoxyphenyl)methyl}-1,1-

dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

872171-49-8 HCAPLUS
Urea, N-[3-[(1,1-dimethyl)-1--[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-1H-pyrazol-5-yl]-N'-(4-fluorophenyl)-(9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 26 Aug 2005 ACCESSION NUMBER: 2005:904352 HCAPLUS DOCUMENT NUMBER: 143:248386

DOCUMENT NUMBER: TITLE:

143:248386
Preparation of substituted azole derivatives for treating diseases mediated by PTPase activity Mjalli, Adnan M. M.; Polisetti, Dharma R.; Subramanian, Govindan; Quada, James C.; Arimilli, Murty N.; Yarragunta, Ravindra R.; Andrews, Robert INVENTOR(S):

C.;

PATENT ASSIGNEE(S): SOURCE:

Xie, Rongyuan
USA
U.S. Pat. Appl. Publ., 204 pp.
CODEN: USXXCO
Patent
English
1

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT:

ATENT	INFO	RMATI	ON:														
		NO.														ATE	
		51872					2005										
		52143															
		1909															
WC		50803															
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE.	GH.	GM.	HR.	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
							LV,										
							PL.										
							ŤZ,										
	DW.	: BW.															
	~"						RU,										
							GR,										
							BF,										
								ы,	CF,	CG,	CI,	CI1,	GA,	GIV,	σų,	GW,	ML,
					TD,							2220			_		
E		0118															
	R:	AT,															
						ŁU,	MC,	ΝĹ,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	AL,	BA,
		HR,	LV,	MK,	YU												
RIORI	TY AP	PLN.	INFO	.:						US 2	004-	5439	71P		P 2	0040	212
										WO 2	005-	US 45	90		W 2	0050	211

MARPAT 143:248386

$$T \xrightarrow{L^{2}, Ar^{2} \xrightarrow{L^{1}} \xrightarrow{L^{1}} \xrightarrow{N} Ar^{1}}$$

AB The title compds. I $\{a, b = 0-2; W = 0, S, NR2 \}$ (wherein R2 = alkyl, etc.); R1 = H, halo, CN, etc.; L1 = a direct bond, (un)substituted NHCO, NHSO2,

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
etc.; Ar1 = (un)substituted (hetero)arylene, fused cycloalkylaryl, etc.; Ar2
= (un)substituted (hetero)arylene, fused arylcycloalkylaryl, etc.; L2 =
CH2, O, alkylene, etc.) which can be useful as inhibitors of protein
tyrosine phosphatases and thus can be useful for the management,
treatment, control, or the adjunct treatment of diseases mediated by
PTPase activity such as type I diabetes and type II diabetes, were prepd.
Thus, treating
4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1Himidazole with Me bromoacetate followed by ester hydrolysis afforded 56%
(4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1Himidazole with Me bromoacetate followed by ester hydrolysis afforded 56%
(4-(2,4-dichlorophenyl)-2-[2-(4-methoxyphenyl)-(E)-vinyl]-1H-inidazol-1yl]acetic acid. The representative compds. I were tested for interior of PTP-1B. In General, the exemplified compds. I were tested for interior of PTP-1B. In General, the exemplified compds. I want inhibit PTP-1B with IC50 of less than 20 µM. The pharmaceutical compns. comprising the compds. I, and their use in treating human or animal disorders are also disclosed.

I861243-91-98 863245-57-2P 863245-74-3P
863246-05-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted arole derivs. for treating diseases

mediated by
PTPS activity)
RN 863243-91-9 HCAPLUS

N1, 25-Thiadiazolidin-3-one, 5-(4-[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl])[1,1'-biphenyl]-4-y-lethenyl]-1H-imidazol-1yl]methyl]phenyl]-4, 4-dimethyl-, 1,1-dioxide (SCI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:continuous} \begin{array}{lll} 863245-57-2 & \text{RCAPLUS} \\ 1,2,5-\text{Thiadiazolidin-3-one, } 5-[4-[[4-(2,4-\text{dichlorophenyl})-2-\{(1E)-2-[3'-(\text{trifluoromethoxy})](1,1'-\text{biphenyl}]-4-yl] \\ \text{ethenyl}]-1.H-\text{imidazol-1-yl}] \\ \text{methyl}] \\ \text{phenyl}]-1,1-\text{dioxide (9CI) (CA INDEX NAME)} \end{array}$

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

663243-80-5P 863243-92-9P 863243-93-0P 863243-94-1P 863244-05-7P 863244-06-6P 863244-07-9P 863244-08-7P 863244-17-1P 863244-51-7P 863244-51-3P 863244-51-3P 863244-51-3P 863244-51-3P 863245-51-4P 863245-56-1P 863246-10-9P 863246-11-1P 863246-11-2P 86324

BBJ207-U3-UF RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of substituted azole derivs. for treating diseases mediated by PTPase activity)
RN 863243-80-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-{(4-(2,4-difluorophenyl)-2-{(1E)-2-{3'-(trifluoromethyl){1,1'-biphenyl}-4-yl]ethenyl}-1H-imidazol-1-yl]methyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

863245-74-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $\label{eq:controller} \begin{array}{lll} 863246-05-3 & \text{MCAPLUS} \\ \text{Benzoic acid}, & 4-\left[4-\left(2,4-\text{dichlorophenyl}\right)-2-\left[\left\{1E\right\}-2-\left[4-\left(1,1-\text{dioxido}-4-\text{oxolity}\right)-2+1\right\}\right] \\ + \left[1,2,5-\text{thiadiazolidin}-2-y1\right] \text{ phenyl}-1 \\ \text{methyl ester (9CI)} & (CA INDEX NAME) \\ \end{array}$

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863243-92-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-[2,4-dichlorophenyl]-2-[(1E)-2-[3'-(trifluoromethyl)]1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-2,4,4-trimethyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863243-93-0 HCAPLUS
1,2,5-Thladiazolidin-3-one, 5-[4-[[4-phenyl-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

PAGE 1-A

863243-94-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2-chlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863244-06-8 HCAPLUS
1,2,5-Thiadlazolidin-3-one, 5-[4-[[4-(3,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-07-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(3,4-difluorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863243-95-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(4-chlorophenyl)-2-[(1E)-2-[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-05-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863244-08-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2-chloro-4-fluorophenyl)-2-[(1E)-2-(3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863244-13-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-{4-{2,4-dichloropheny1}-2-{3'-(methylsulfony1)[1,1'-bipheny1]-4-y1]methyl]-1H-imidazol-1-y1]pheny1]-,
1,1-dioxide {9C1} (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-51-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[2-[4-

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863244-53-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[2-[3'-(trifluoromethoxy](1,1'-bipheny1]-4-y1]ethy1]-1H-imidazol-1-y1]methy1]pheny1}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863245-25-4 HCAPLUS CN Benzoic acid, 4-[[4-{2,4-dichlorophenyl}-2-[{1E}-2-[3'-(1,1-dioxido-4-oxoL4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (trifluoromethyl)phenyl)ethyl)-1H-imidazol-1-yl)methyl)phenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 863244-52-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4-[[4-(2,4-dichlorophenyl)-2-[2-[2-fluoro-4(trifluoromethyl)]henyl|ethyl)l=H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA IMDEN NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl)ethenyl]-1H-imidazol-1yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-56-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(2-[(1E)-2-[3',5'-bis(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-58-3 HCAPLUS
(1,2,5-Thiaddazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(Z'-fluoro-5'-propoxy[1,1'-biphenyl]-4-yl)ethenyl]-IH-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[[2-{(1E)-2-(3'-chloro[1,1'-biphenyl]-4-y1)ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-60-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[3'-(1-

methylethoxy){1,1'-biphenyl}-4-yl}ethenyl}-1H-imidazol-1-yl}methyl}phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Double bond geometry as shown.

RN 863245-63-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dimethylethyl)-5'-methyl[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-64-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[(2-[(1E)-2-(4-(5-chloro-2-thienyl)phenyl)]tethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-61-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4'[(1-methylethyl)thio][1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-62-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 863245-66-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-[[2-[(1E)-2-[4-(5-acetyl-2-thienyl)phenyl]ethenyl]-4-(2,4-dichlorophenyl)-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-67-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2'-fluoro-5'-[trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863245-68-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-{2,4-dichloropheny1}-2-{(1E)-2-[3'3,3-dimethylbutoxy)[1,1'-bipheny1]-4-y1]etheny1]-1H-imidazol-1y1]methy1]pheny1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-69-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(4,4,4-trifluorobutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9Cl) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

863245-72-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[{4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl][1,1'-biphenyl]-4-yl]ethenyl]-H-inidazol-1-yl]methyl]phenyl]-4-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

863245-75-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[2-

fluoro-4-(trifluoromethyl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]2-methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

 $\begin{array}{lll} 863245-70-9 & \text{RCAPLUS} \\ 1,2,5-\text{Thiadiazolidin-3-one,} & 5-\{4-[\{4-(2,4-\text{dichloropheny1}\}-2-[\{1E\}-2-\{3'-1\}]\} \\ \end{array}$

fluoro-4'-(4,4,4-trifluorobutoxy)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA:INDEX NAME)

Double bond geometry as shown.

863245-71-0 HCAPLUS
Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2-yl]ethenyl]-4-fluoro[1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

863245-78-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4-(4,4,4-trifluorobutoxy)phenyl]-thenyl]-lH-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863245-80-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[4-[4-

(1,1-dimethylethyl)phenoxy]phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl}, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863245-82-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichloropheny1)-2-[(1E)-2-[4-[4-

(trifluoromethyl)phenoxy]phenyl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-03-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[4-(2,4-dichlorophenyl)-2-{(1E)-2-[3'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-inidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Double bond geometry as shown.

RN 863246-09-7 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-[2,4-dichlorophenyl]]-1-[[4-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]=1H-imidazol-2-yl]ethenyl][1,1'-biphenyl]-3-yl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Double bond geometry as shown.

RN 863246-04-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-{(1E)-2-[4-(2,4-dichlorophenyl)-1-ethyl-1H-imidazol-2-yl]ethenyl]phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-06-4 HCAPLUS
CN Benzoic acid, 4-[(4-(2,4-dichlorophenyl)-2-[(1E)-2-[4-(1,1-dioxido-4-oxo-1,Z,5-thiadiazolidin-2-yl)phenyl]ethenyl]-1H-imidazol-1-yl]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 863246-10-0 HCAPLUS
CN Carbamic acid, [4'-[(1E)-2-[4-(2,4-dichlorophenyl)-1-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]-1H-imidazol-2yl]ethenyl][1,1'-biphenyl]-3-yl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 863246-11-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-{1-

methylethyl) [1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl], 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-12-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-(3'-methyl[1,1'-biphenyl]-4-yl)ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $863246-13-3 \quad HCAPLUS \\ 1,2,5-Thiadiazolidin-3-one, \quad 5-[4-\{[4-(2,4-dichlorophenyl)-2-[(1E)-2-(4-phenoxyphenyl]-th-imidazol-1-yl]methyl]phenyl]-, \quad 1,1-dioxide$ (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Double bond geometry as shown. (Continued)

863287-03-0 HCAPLUS 1,2,5-Thiaddazolidin-3-one, 5-[4-[[4-(2,6-dichlorophenyl)-2-[(1E)-2-[3'-trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

IT 863247-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Reactant or reagent)
mediated by
PTPase activity)
RN 863247-41-0 HCAPLUS
CN Benzoic acid,
4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-(1,1-dioxido-4-oxo-

L4 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

863246-15-5 HCAPLUS 1,2,5-Thiediazolidin-3-one, 5-[4-[[4-(2,4-dichlorophenyl)-2-[(1E)-2-[3'-

(trifluoromethyl)[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]-2-methylphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

 $863246-16-6 \quad HCAPLUS \\ 1,2,5-Thiadiazolidin-3-one, 5-\{4-[\{4-\{2,4-dichlorophenyl\}-2-\{\{1E\}-2-\{3'-trifluoromethyl\}[1,1'-biphenyl]-4-yl]ethenyl]-1H-imidazol-1-yl]methyl]phenyl]-4-propyl-, 1,1-dioxide (9CI) (CA INDEX NAME)$

ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]-H-imidazol-1-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 03 May 2005 ACCESSION NUMBER: 2005:378875 HCAPLUS DOCUMENT NUMBER: 143:19267 HCAPLUS Structure-based design of protein and protein access to the state of the

ACCESSION NUMBER: 2005:378875 HCAPLUS

DOCUMENT NUMBER: 143:19267

AUTHOR(S): Structure-based design of protein tyrosine phosphatase-1B inhibitors

AUTHOR(S): Black, Emma: Breed, Jason; Breeze, Alexander L.; Embrey, Kevin; Garcia, Robert: Gero, Thomas W.; Godfrey, Linda; Kenny, Peter W.; Morley, Andrew D.; Minshull, Claire A.; Pannifer, Andrew D.; Read, Jon; Rees, Amanda; Russell, Daniel J.; Toader, Dorin; Tucker, Julie

CORPORATE SOURCE: AstraZeneca, Cheshire, SK10 4TG, UK
BOURCE: Bioorganic 4 Medicinal Chemistry Letters (2005), 15(10), 2503-2507

CODEN: BMCLES; ISSN: 0960-894X

PUBLISHER: DOCUMENT TYPE: Journal
LANGUAGE: CASREACT 143:19267

AB Using structure-based design, a new class of inhibitors of protein tyrosine phosphatase-1B (PPTB) has been identified, which incorporate the

1,2,5-thiadiarolidin-3-one-1,1-dioxide template.
692765-80-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-based design of protein tyrosine phosphatase-1B inhibitors)
692765-80-3 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-44-6P 692764-89-9P 692764-94-6P 852835-44-0P 852835-45-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (structure-based design of protein tyrosine phosphatase-1B inhibitors) 612530-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852835-45-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2-methoxyphenyl)-, 1,1-dioxide (9CI) (CA

REFERENCE COUNT: THIS

THERE ARE 22 CITED REFERENCES AVAILABLE FOR

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-89-9 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

692764-94-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

852835-44-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-methylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2005
ACCESSION NUMBER: 2005:347030 HCAPLUS
DOCUMENT NUMBER: 142:411350

TITLE: Preparation of 1-oxo and 1,1-dioxoisothiszolone and related modulators of proteins such as phosphatases that bind phosphorylated peptides and proteins

Combs, Andrew P.; Yue, Eddy Wai Tsun; Bower, Michael Jason; Zhu, Wenyu; Crawley, Matthew Lentz; Sparks, Richard Bruce; Pruitt, James Russell; Takvorian, Amy

PATENT ASSIGNEE(S): CODEN: PIXKD2

POCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO. WO 2005035551							DATE			APPL	ICAT	ION	NO.		DATE				
								2005	0421		WO 2	004-1	US 3 3	212		2	0041	007		
	WO	2005	0355	51		A3		2006	0908											
		W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,		
			CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	15,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,		
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,		
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
			TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	υG,	ZM,	ZW,	AM,		
			AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
			EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,		
			SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,		
			SN,	TD,	TG															
	บร	2005	2727	78		A1		2005	1208		US 2	004-	9603	44		2	0041	007		
	UŞ	7141	596			В2		2006	1128											
101	RITY	APP	LN.	INFO	. :						US 2	003-	5100	02 P		P 2	0031	008		
											US 2	003-	5293	72 P		P 2	0031	211		
											US 2	004-	6005	06P		P 2	0040	811		

OTHER SOURCE(S):

CASREACT 142:411350; MARPAT 142:411350

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention provides 1-oxo and 1,1-dioxoisothiazolones (shown

I-IV; also isothiazolidinone analogs of I-IV with R16 and R17 in place of R15 and Rz as a substituent at the 5 position of the isothiazolidinone ring; variables defined below; e.g. V) and related compds. that can modulate (no data) the activity of a target protein, such as a phosphatase, that selectively binds phosphorylated peptides or proteins. The present compds. can be useful (no data) in treating diseases or disorders, including, for example, diabetes and obesity, that are connected directly or indirectly to the activity of the target protein. Methods of preparation are claimed and hundreds of example prepns. are included. For example, V was prepared in 12 steps (50, 62, 100, 59, not

- ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) detd., 100, 100, 99, not detd., not detd., 43, and 25 % yield) starting from N-tert-butyl-3-[2-(tert-butylcarbamoyl)ethyldisulfanyl]propionamide. For I-IV: a dashed line indicates an optional bond; Scl is a 1st mol. scaffold or is absent; Sc2 is a 2nd mol. scaffold or is absent, wherein
- least one of Sc1 and Sc2 is present; or Sc1 and Sc2 together with X1 and X2 or X4 and X5 form a 5-, 6-, or 7-membered fused carbocyclic ring or a 5-, 6-, or 7-membered fused heterocarbocyclic ring; X1 is C or N when Sc1 is present; X1 is CR1, N, NR2, CO, CS, SO, or SO2 when Sc1 is absent; X2 is C or N when Sc1 is present; X2 is C or N when Sc2 is present; X2 is C or N when Sc2 is present; X2 is C or N when Sc2 is present; X2 is C or N, N, NR2, CO, CS, SO, or SO2 when Sc2 is absent; X3 is C or N; each D1, D2, and D3 = CR1, N, NR2, CO, CS, SO, or SO2, wherein the ring formed by X1, X2, X3, D1, D2, and D3 is an arom. ring; X4 is C or N when Sc1 is present; X4 is O, S, CR3, N, NR4,
- CS, SO, or SO2 when Sc1 is absent; X5 is C or N when Sc2 is present; X5
- O, S, CR3, N, NR4, CO, CS, SO, or SO2 when Sc2 is absent; X6 is C or N. Each E1 and E2 = O, S, CR3, N, NR4, CO, CS, SO, or SO2, wherein the rin formed by X4, X5, X6, E1, and E2 is an aron. ring; Rz is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl, OR26, SR28, NO2, CN, SOR29, SOR29, COR30, COR031, NR32R33, a 5- or 6-membered heterocarbocyclyl group, or tetrazolyl. R15 is H, halo, C1-C4 alkyl, C3-C6 cycloalkyl, haloalkyl,
- OH,

 C1-C4 alkoxy, C1-C4 haloalkoxy, SH, C1-C4-chioalkoxy, CN, NO2, SO(C1-C4
 alkyl), SO(C1-C4 haloalkyl), SO(C3-C6 cycloalkyl), SONN2, SO3H, SO2(C1-C4
 alkyl), SO(C1-C4 haloalkyl), SO(C3-C6 cycloalkyl), SONN2, SO3H, SO2(C1-C4
 alkyl), SO2(C1-C4 haloalkyl), SO2(C3-C6 cycloalkyl), SO2NH2, CHO, COOH,
 CO(C1-C4 alkyl), CO(C1-C4 cycloalkyl), COC(C1-C4 haloalkyl),
 CO(heterocarbocyclyl), COO(C1-C4 alkyl), COO(C1-C4 haloalkyl),
 CONHC3-C5 cycloalkyl), CON(C1-C4 alkyl), CON(C1-C4 alkyl), CONHC3-C6
 cycloalkyl), CONHC3-C6 cycloalkyl), OR N(C1-C4 alkyl), NH(C1-C4
 alkyl), NH(C3-C6 cycloalkyl), NH(C3-C6 cycloalkyl), CON(C1-C4
 haloalkoxy, SH, C1-C4 thioalkoxy, CN, NO2, SO(C1-C4 alkyl), SO(C1-C4
 haloalkyl), SO2(C1-C6 cycloalkyl), SONN2, SO3H, SO2(C1-C4 alkyl), SO(C1-C4
 haloalkyl), SO2(C3-C6 cycloalkyl), SO2(C1-C4
 haloalkyl), SO2(C3-C6 cycloalkyl), SO2NN2, SO3H, SO2(C1-C4
- SO2(C1-C4
 haloalkyl), SO2(C3-C6 cycloalkyl), SO2NH2, CHO, COOH, CO(C1-C4 alkyl),
 CO(C3-C6 cycloalkyl), CO(C1-C4 haloalkyl), CO(heterocarbocyclyl),
 COO(C1-C4 alkyl), COO(C1-C4 alkyl), COO(C1-C4 haloalkyl), COO(C1-C4 cycloalkyl), CON(C3-C6 cycloalkyl), CON(C1-C4 alkyl), CON(C1-C6 eycloalkyl), CON(C3-C6 cycloalkyl),
 ON (C3-C6 cycloalkyl),
 or N(C3-C6 cycloalkyl),
 or N(C3-C6 cycloalkyl),
 they are attached form a C3-C6 cycloalkyl group or a 3-7 membered heterocycloalkyl group; and ql is 1 or 2; addnl. details are given in the claims.
- networkstand, recommended the control of the contro
- phenylpropionyl]amino]-N-pentyl-3-{4-{1,1,4-trioxo{1,2,5}} thiadiazolidin-2-yl)phenyl|propionamide 850315-24-1P, N-{(15)-2-{4-{1,1-Dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl}-1-{5-{trifluoromethyl}-1H-benzimidazol-2-yl]ethyl|biphenyl-4-sulfonamide 850315-36-5P 850315-40-1P, 4-Bromo-N-{(15)-2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl]-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-2-thiadiazolidin-2-yl)phenyl-1-{5-{trifluoromethyl}-1H-benzimidazol-
- ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 850327-93-4P, N-{(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl|ethyl|3-chlorobenzenesulfonamide trifluoroacetate 850327-95-6P, N-{(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl|ethyl|-3-fluorobenzenesulfonamide trifluoroacetate RL: PAC (Pharmacological activity); SPN (Synthetic preparation); TNU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 - (drug candidate; prepn. of 1-oxo and 1,1-dioxoisothiazolone and
- modulators of proteins such as phosphatases that bind phosphorylated
 peptides and proteins)
 80-151-19-4 NCAPLUS
 L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.

- 850315-22-9 HCAPLUS L-Phenylalaninamide, N-{(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-{1,1-dioxidod-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- 850315-24-1 HCAPLUS
 [1,1'-Biphenyl]-4-sulfonamide, N-[{15}-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]- (9CI) (CA INDEX NAME)

- ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-44-5p, N-([15])-2-(4-1[1.-Dioxid-0-4-0xo-1.2],5-thiadizarolidin-2-yl)phenyl]-1-[5-(trifluoromethyl]-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoromethyl)benzenesulfonamide trifluoroacetate 850315-89-9p, N-([15])-2-(4-1[1.-Dioxid-0-4-0xo-1.2],5-thiadiazolidin-2-yl)phenyl]-1[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxyl)benzenesulfonamide trifluoroacetate 850315-63-8p, N-[(15)-2-(3-thiadiazolidin-2-yl)phenyl]-1[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]biphenyl-4-sulfonamide trifluoroacetate 850315-65-0P 850315-69-4P
- 4-Bromo-N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-2-(trifluoromethoxy)benzenesulfonamide trifluoroacetate 850315-73-0P, N-[(1S)-2-[3-Chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bis(trifluoroacethyl)benzenesulfonamide trifluoroacetate 850327-65-0P 850327-67-2P, N-[(1S)-1-(5-Chloro-1H-
- benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-69-49, N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl}-4-cyanobenzenesulfonamide trifluoroacetate 850327-71-8P,
- N-[(1S)-1-(5-Chloro-1H-benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]pheny1]ethy1]-3-phenoxybenzenesulfonamide trifluoroacetate 650327-73-0P, N-[(1S)-1-(5-Chloro-1H-
- benzimidasol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)phenyl)ethyl]-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-75-2P, N-[(13)-1-(5-Chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-77-4P, N-[(15)-1-(1N-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-79-6P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyanobenzenesulfonamide trifluoroacetate 850327-81-0P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide trifluoroacetate 850327-83-2P, N-[(15)-1-(1H-Benzimidazol-2-yl)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyanobenzenesulfonamide
- 2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3-phenoxybenzenesulfonamide trifluoroacetate 850327-85-49,
 N-[(15)-1-(1H-Benzimidazol-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3,4-dimethoxybenzenesulfonamide trifluoroacetate 850327-87-69, N-[(15)-1-(1H-Benzimidazol-2-y1)-2-(3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl]ethyl]-3,5-dimethylbenzenesulfonamide trifluoroacetate 850327-89-89,
 3-Chloro-N-[(15)-1-(5-chloro-1H-benzimidazol-2-y1)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)]phenyl]ethyl]benzenesulfonamide trifluoroacetate 850327-91-29, N-[(15)-1-(5-chloro-1H-
- benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-fluorobenzenesulfonamide trifluoroacetate

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- RN 850315-36-5 HCAPLUS
 CN Benzenesulfonamide,

 y1[15]-2-[4-{1, 1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]ethyl]-4(trifluoromethyl)-1H-benzimidazol-2-y1]ethyl]-4-

 - CRN 850315-35-4 CMF C25 H19 F6 N5 O5 S2
- Absolute stereochemistry.

- CM 2
- CRN 76-05-1 CMF C2 H F3 O2

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-40-1 HCAPLUS
Benzenesulfonamide, 4-bromo-N-[(1S)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-39-8 CMF C25 H18 Br F6 N5 O6 S2

Absolute stereochemistry.

RN 850315-44-5 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-2-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-63-8 HCAPLUS
[1,1'-Biphenyl]-4-sulfonamide, N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-

1,2,5-thiadiazolidin-2-yl)phenyl]-1-{5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-62-7 CMF C30 H23 C1 F3 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) yl)phenyl)-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl]-3,5-bia(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-43-4 CMF C26 H18 F9 N5 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

Absolute stereochemistry.

RN 850315-48-9 HCAPLUS
CN Benzenesulfonamide,
N-{(15)-2-[4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-{5-(trifluoromethyl)-1H-benzimidazol-2-yl]ethyl}-2(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-47-8 CMF C25 H19 F6 N5 O6 S2

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CM 2

-со2н

850315-65-0 HCAPLUS
Benzenesulfonamide, N-[{1S}-2-{3-chloro-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-{5-(trifluoromethyl)-1R-benzimidazol-2-yl)ethyl]-4-(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850315-64-9 CMF C25 H18 C1 F6 N5 O5 S2

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 850315-69-4 HCAPLUS
CN Benzenesulfonamide,
4-bromo-N-[(15)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-2-(trifluoromethoxy)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

СМ 1-

CRN 850315-68-3 CMF C25 H17 Br C1 F6 N5 O6 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

СМ 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-65-0 HCAPLUS

Benzenesulfonamide,
N-{(iS)-1-{S-chloro-1H-benzimidazol-2-yl}-2-{3-chloro-4-(l,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenyl]ethyl]-,
mono(trifluoroacetate) {9CI} (CA INDEX NAME)

CM 1

CRN 850327-64-9 CMF C23 H19 C12 N5 O5 S2

Absolute stereochemistry.

CM 2

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850315-73-0 HCAPLUS
Benzenesulfonamide, N-[(1S)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]-1-[5-(trifluoromethyl)-1H-benzimidazol-2-yl)ethyl]-3,5-bis(trifluoromethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850315-72-9 CMF C26 H17 C1 F9 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN.

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-67-2 HCAPLUS
CN Benzenesulfonamide,
N-[[IS]-1-(S-chloro-lH-benzimidazol-2-yl)-2-[3-chloro4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-2-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-66-1 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-69-4 HCAPLUS
CN Benzenesulfonamide,
N-[(15)-1-[5-chloro-lH-benzimidazol-2-yl)-2-[3-chloro4-[1]-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-4-cyano-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

см 1

CRN 850327-68-3 CMF C24 H18 C12 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

CM 1

CRN 850327-70-7 CMF C29 H23 C12 N5 O6 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-75-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-74-1 CMF C25 H23 C12 N5 O5 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 850327-73-0 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-

4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)ethyl)-3,4-dimethoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-72-9 CMF C25 H23 C12 N5 O7 S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

г— c—со₂н

850327-77-4 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiediazolidin-2-yl)phenyl]ethyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-76-3 CMF C23 H20 C1 N5 O5 S2

Absolute stereochemistry.

CRN 76-05-1

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CMF C2 H F3 O2 (Continued)

850327-79-6 HCAPLUS
Benzenesulfonamide, N-[(1s)-1-(1H-benzimidazo1-2-y1)-2-[3-chloro-4-(1,1-dioxido4-4-oxo-1,2,5-thiadiazolidin-2-y1)pheny1]ethy1]-2-cyano-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-78-5 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

2

850327-81-0 HCAPLUS
Benzenesulfonamide, N-{(1S)-1-(1H-benzimidazo1-2-yl)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazo1idin-2-yl)phenyl]ethyl}-4-cyano-,
mono(trifluoroacetate) (9C1) {CA INDEX NAME}

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

2 CM

CRN 76-05-1 CMF C2 H F3 O2

850327-85-4 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,4-dimethoxy-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-84-3 CMF C25 H24 C1 N5 07 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM 1 (Continued)

CRN 850327-80-9 CMF C24 H19 C1 N6 O5 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

-со2н

850327-83-2 HCAPLUS
Benzenesuifonamide, N-{(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-0xo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-phenoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-82-1 CMF C29 H24 C1 N5 O6 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850327-87-6 HCAPLUS
Benzenesulfonamide, N-[(1S)-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3,5-dimethyl-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-86-5 CMF C25 H24 C1 N5 O5 S2

Absolute stereochemistry

CM 2

850327-89-8 HCAPLUS
Benzenesulfonamide, 3-chloro-N-[(15)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)phenyl]ethyl]-,

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN mono(trifluoroacetate) (9CI) (CA INDEX NAME) (Continued)

CM 1

CRN 850327-88-7 CMF C23 H18 C13 N5 O5 S2

Absolute stereochemistry.

2

CRN 76-05-1 CMF C2 H F3 O2

RN 850327-91-2 HCAPLUS
CN Benzenesulfonamide,
N-[(1S)-1-(5-chloro-1H-benzimidazol-2-yl)-2-[3-chloro4-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin-2-yl)phenyl]ethyl]-3-fluoro-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-90-1 CMF C23 H18 C12 F N5 O5 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

-CO2H

850327-95-6 HCAPLUS
Benzenesulfonamide, N-{(1S}-1-(1H-benzimidazol-2-yl)-2-[3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]-3-fluoro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 850327-94-5 CMF C23 H19 Cl F N5 OS S2

Absolute stereochemistry.

L4 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

850327-93-4 HCAPLUS
Benzenesulfonamide, N-{(15)-1-(1H-benzimidazol-2-y1)-2-{3-chloro-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)phenyl}ethyl}-3-chloro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 850327-92-3 CMF C23 H19 C12 N5 O5 S2

Absolute stereochemistry.

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

CO2H

IT 850315-20-7P, [(S)-2-[4-(5-Benzyl-1,1,4-

IT 850315-20-7P, {(5)-2-(4-(5-Benzyl-1,1,4trioxo(1,2,5)thiadiazolidin-2-yl)phenyl]-1-(pentylcarbamoyl)ethyl]carbamic
acid tert-butyl ester 850315-21-8P, {(15)-1-[(15)-2-(4-(5Benzyl-1,1,4-trioxo(1,2,5)thiadiazolidin-2-yl)phenyl]-1(pentylcarbamoyl)ethyl]carbamoyl]-2-phenylethyl]carbamic acid tert-butyl
ester 850315-23-0P, (2S)-3-[4-(5-Benzyl-1,1,4trioxo(1,2,5)thiadiazolidin-2-yl)phenyl]-2-[(2S)-2-([2-(4methoxyphenyl)acetyl]amino]-3-phenylpropionyl]amino]-N-pentylpropionamide
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation of 1-oxo and 1,1-dioxoisothiazolne and related
modulators of

proteins such as phosphatases that bind phosphorylated peptides and
proteins)
RN 850315-20-7 HCAPLUS
CArbamic acid, ([15)-1-[4-[1,1-dioxido-4-oxo-5-(phenylmethyl]-1,2,5thiadiazolidin-2-yl]phenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (SCI) (CA INDEX NAME)

Absolute stereochemistry.

850315-21-8 HCAPLUS L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl-(9CI) (CA INDEX NAME)

ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

850315-23-0 HCAPLUS L-Phenylalaninamide, N-[(4-methoxyphenyl)acetyl]-L-phenylalanyl-4-[1,1-dioxido-4-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612528-23-1P 612529-46-1P 612530-69-5P 852335-50-0P 852358-51-1P 8523358-53-3P 852358-54-4P 852358-56-6P 852358-57-7P RL: SPN (Synthetic preparation) PREP (Preparation) (preparation of sulfonylhydantoins via reaction of amino acid esters

sulfamide and DBU) 612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2-CH2-Ph

612529-46-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-bromophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2-Ph

RN CN (9CI) 852358-50-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-, 1,1-dioxide (CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 11 Apr 2005 ACCESSION NUMBER: 2005:308290 HCAPLUS DOCUMENT NUMBER: 143:7658

DOCUMENT NUMBER: TITLE:

AUTHOR(S): CORPORATE SOURCE:

143:7658
Expedient syntheses of sulfonylhydantoins and two
six-membered analogs
Campbell, Andrew D.: Birch, Alan M.
Research and Development, AstraZeneca, Cheshire, SK10
APC 11V Research and Development, Astron. 4TG, UK Synlett (2005), (5), 834-838 COODEN: SYNLES; ISSN: 0936-5214 Georg Thieme Verlag Journal English CASREACT 143:7658

SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

A range of α -amino esters can be turned into sulfonylhydantoins in a single, atom-economic step using sulfamide and DBU. E.g., reaction of BNHKCH2CO2Ct with sulfamide and DBU gave 65% sulfonylhydantoin I. This procedure obviates the need for a three- or four-step sequence utilized

traditional procedures. Two new six-membered analogs [5-aryl-1,2,6-thiadiazinan-3-one 1,1-dioxides and 5-aryl-1,2-thiazinan-3-one 1,1-dioxides), e.g. II and III, have also been prepared utilizing novel synthetic protocols.

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-51-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(2-methoxyphenyl)methyl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

852358-53-3 HCAPLUS
Benzonitrile, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-(9CI) (CA INDEX NAME)

852358-54-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
ethyl ester (9CI) (CA INDEX NAME)

ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

852358-56-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-([1,1'-biphenyl]-3-ylmethyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)

852358-57-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-methyl-5-(phenylmethyl)-, 1,1-dioxide, (45)

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 08 Mar 2005
ACCESSION NUMBER: 2005:202894 HCAPLUS DOCUMENT NUMBER: 142:366767

ACCESSION NUMBER: 2005:202894 HCAPLUS
DOCUMENT NUMBER: 142:366767
ITITLE: 1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides are potent inhibitors of human tryptase
AUTHOR(S): Wong, Tzutshin; Groutas, Christopher S.; Mohan, Svath; Lai, Zhong; Alliston, Kevin R.; Vu, Ngs; Schechter, Norman M.; Groutas, William C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Archives of Biochemistry and Biophysics (2005), 436(1), 1-7
CODEN: ABBITA; ISSN: 0003-9861

LINGUAGE: English
AB The authors describe herein the design, synthesis, and in vitro biochem. evaluation of a series of potent, time-dependent inhibitors of the mast cell-derived serine protease tryptase. The inhibitors were readily obtained by attaching various heterocyclic thiols, as well as a basic primary specificity residue Pl, to the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold. The inhibitors were found to be devoid of any inhibitory activity toward a neutral (elastase) or cysteine (papain) protease, however they were also fairly efficient inhibitors of bovine trypsin. The differential inhibition observed with trypsin suggests that enzyme selectivity can be optimized by exploiting differences in the S' substess of the two enzymes. The results described herein demonstrate the

versatility of the heterocyclic scaffold in fashioning mechanism-based inhibitors of neutral, basic, and acidic (chymo)trypsin-like serine proteases. 849415-30-1P 849415-31-2P 849415-32-3P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea) ΙT

(1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

potent inhibitors of human tryptase)
649415-30-1 HCAPLUS
1,2,5-Thladiazolidin-3-one, 4-(4-aminobuty1)-2-[(2-benzoxazolylthio)methy1)-5-(phenylmethy1)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-31-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2-[{{5-phenyl-1,3,4-oxadiazol-2-yl}thio]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Absolute stereochemistry.

849415-32-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{4-aminobutyl}-5-(phenylmethyl)-2-[{(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-24-3P 849415-25-4P 849415-26-5P 849415-27-6P 849415-28-7P 849415-29-8P RL: RCT (Reactant); SPR (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (1,2,5-Thiadiazolidin-3-one 1,1-dioxide-based heterocyclic sulfides

are

potent inhibitors of human tryptase)
849415-24-3 RCAPLUS
Carbamic acid, [4-{(3S)-1,1-dioxido-4-oxo-2-(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

849415-25-4 HCAPLUS
Carbamic acid, [4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-26-5 HCAPLUS
Carbamic acid, {4-{(3S)-5-(chloromethyl}-1,1-dioxido-4-oxo-2-(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 849415-27-6 HCAPLUS
CN Carbamic acid,
[4-{(35)-5-(2-benzoxazolylthio)methyl}-1,1-dioxido-4-oxo-2(phenylmethyl)-1,2,5-thiadiazolidin-3-yl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

THERE ARE 32 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L4 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

849415-28-7 HCAPLUS
Carbamic acid, {4-{(3S)-1,1-dioxido-4-oxo-2-{phenylmethyl)-5-{{(5-phenyl-1,3,4-oxdiazol-2-yl)thio|methyl}-1,2,5-thiadiazolidin-3-yl}butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

849415-29-8 HCAPLUS
Carbamic acid, {4-[(35)-1,1-dioxido-4-oxo-2-(phenylmethyl)-5-[[(3-phenyl-1,2,4-oxdiazol-5-yl)thio]methyl)-1,2,5-thiadiazolidin-3-yl]butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 19 Aug 2004 ACCESSION NUMBER: 2004:677210 HCAPLUS

DOCUMENT NUMBER:

TITLE:

141:235669
Potent inhibition of human leukocyte elastase by 1,2,5-thiadiazolidin-3-one 1,1 dioxide-based sulfonamide derivatives
Lai, Zhong, Can, Xiangdong, Wei, Liuqing, Alliston, Kevin R., Yu, Hongyl, Li, Yue H., Groutas, William C. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Archives of Biochemistry and Biophysics (2004), 429(2), 191-197
CODEN: ABBIA4; ISSN: 0003-9861
Elsevier
Journal AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

Journal English CASREACT 141:235669 OTHER SOURCE(S):

R SOURCE(S): CASREAT 141:235669
The design, synthesis, and in vitro biochem. evaluation of a class of mechanism-based inhibitors of human leukocyte elastase (HLE) that incorporate in their structure a 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold with appropriate recognition and reactivity elements appended to it is described. The synthesized compds. were found to be efficient, time-dependent inhibitors of HLE. The interaction of the inhibitors with HLE is postulated to lead to the formation of a highly reactive lfonul

N-sulfonyl
imine (a Michael acceptor) that arises from an enzyme-induced sulfonamide
fragmentation cascade. Subsequent reaction ultimately leads to the
formation of a relatively stable acyl enzyme. The results cited herein
demonstrate convincingly the superiority of the
1,2,5-thiadiarolidin-3-one
1,2,5-thiadiarolidin-3-one

- insularoildin-3-one 1.1 dioxide scaffold over other scaffolds (e.g., saccharin) in the design of inhibitors of (chymo)tryppin-11ke serine proteases. 749866-31-79 749866-32-09 749866-33-99 749866-34-09

749866-34-0P
RI: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(potent inhibition of human leukocyte elastase by 1,2,5-thiadiazolidin-

5-thiadiazolidin-3-one l,1-dioxide-based sulfonamide derivs.) 749866-31-7 HCAPLUS L-Phenylalanine, N-[[[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-32-8 HCAPLUS D-Phenylalanine, N-[[[(48)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STM (Continued) (phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-33-9 HCAPLUS
L-Phenylalanine, N-[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

749866-34-0 HCAPLUS L-Phenylalanine, N-[{[(4s)-4-{2-methylpropyl})-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl)- (9CI) INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 212331-99-2P 749866-30-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by 1,2,5-thiadiazolidin-

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: THIS

THERE ARE 36 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 3-one 1,1-dioxide-based sulfonamide derivs.)
212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

749866-30-6 HCAPLUS Ethanethioic acid, S-{{{45}}-4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-{phenylmethyl}-1,2,5-thiadiazolidin-2-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 220869-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(potent inhibition of human leukocyte elastase by

1,2,5-thiadiazolidin3-one 1,1-dioxide-based sulfonamide derivs.)
RN 220869-64-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 30 Jul 2004

ACCESSION NUMBER: 2004:610081 HCAPLUS

DOCUMENT NUMBER: 141:157120

TITLE: Preparation of sulfahydantoins as phosphate isosteres for use as phosphatase inhibitors in the treatment of cancer and autoimmune disorders

INVENTOR(S): Saunders, Jeffrey O.; Miknis, Gregory F.; Blake, James

INVENTOR(S): James

P.
Vertex Pharmaceuticals Incorporated, USA
PCT Int. Appl., 62 pp.
CODEN: PIXXD2
Patent
English 1
1 PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

-																	
PAT	CENT :	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
						-									-		
WO	2004	0626	64		A1		2004	0729		WO 2	003-	US 4 1	630		2	0031	230
	w:	AE.	AG.	AL.	AM.	AT,	AU,	AZ,	BA;	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN
							DK,										
							IN.										
							MD,										
							SE,										
							ZA,			,	,	•,	,	,			
	DAT.						MW,			5.1	57	77	uc	2 M	7W	ма	
	RW.						TJ,										
							HU,										
		TR,	BF,	ы,	CF,	ÇG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	mk,	NE,	5N,	1.
rG .																	
	2511																
	2003															0031	
	2004																
EP	1594																
	R:						ES,										P'
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	ΗU,	5K	
JP	2006	5149	60		T		2006	0518		JP 2	004-	5666	41		2	0031	23
RIORITY																0021	
										WO 2	003-	0841	630		w 2	0031	230

OTHER SOURCE(S): MARPAT 141:157120

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

AB The invention relates to compds. having a sulfahydantoin or a reverse sulfahydantoin moiety (I) and (II) or pharmaceutically acceptable salts thereof (0 = each (un)substituted C1-8 aliphatic group, C6-10 aryl, heteroaryl having 5-10 ring atoms, heterocyclyl having 3-10 ring atoms; T = C1-6 alkylidene chain wherein one or two nonadjacent methylene units of T are optionally and independently replaced by O, MR, S, CO, CONR, NRCO, NRCOR, SO, SO2, NRSO2, SO2WR, or NRSO2WR; m = 0.1; X = CH2, CO, CT2; R = H or (un)substituted C1-8 aliphatic group or two R groups bound to the

nitrogen are taken together with the nitrogen to form a 3-7 membered heterocyclic ring having 0-2 heteroatoms in addition to the nitrogen

wherein
said heteroatoms are independently selected from N, O, or S), uses
thereof, and related methods. These compds. are inhibitors of
phosphatases, particularly inhibitors of protein tyrosine phosphatase
SHP-2 and are used in the treatment of various phosphatase mediated
diseases such as proliferative diseases, autoimmune disorders, angiogenic
disorders, and cancer. The autoimmune disease is selected from
glomerulonephritis, rheumatoid arthritis, systemic lupus erythematosus,
scleroderma, chronic thyroliditis, Graves' disease, autoimmune gastritis,
diabetes, autoimmune hemolytic anemia, autoimmune neutropenia,
thrombocytopenia, atopic dermatitis, chronic active hepatitis, myasthenia
gravis, multiple sclerosis, infilammatory bowel disease, ulcerative
colitis, Crohn's disease, psoriasis, or graft vs. host disease. The
proliferative disease is selected from acute myelogenous leukemia,
chronic

proliterative disease is selected from acute myelogenous leukemia, mic myelogenous leukemia, metastatic melanoma, Kaposi's sarcoma, multiple myeloma, and HTLV-1-mediated tumorigenesis. The angiogenic disorder is selected from solid tumors, ocular neovasculization, and infantile haemangiomas. The cancer is selected from colon, breast, stomach, and ovarian cancer. Thus, N-alkylation of Me 4-minobenzoate by Et bromoacetate in the presence of EtN at 60° for 2.5 days gave 4-[[(Ethoxycarbonyl]methyl]amino]benzoic acid Me ester which underwent N-sulfamoylation by sulfamoyl chloride in the presence of EtN in CHXCl2 at room temperature overnight to give 4-[N-[(Ethoxycarbonyl)methyl]-N-sulfamoylamino]benzoic acid Me ester (III). Cyclization of III by treatment with NaOMe/MeOH at room temperature overnight gave 4-[1,1,4+trioxo-1,2,5-thiadiazolidin-2-yl)benzoic acid Me ester (IV). IV showed ICSO of 1.0-100 µM against protein tyrosine phosphatase SHP-2. 612527-99-8P 612530-69-5P 729600-44-6P,

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 729600-47-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 729600-48-0 HCAPLUS
CN Benzoic acid, 3-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
methyl ester (9C1) (CA INDEX NAME)

RN 729600+49-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3-phenyl-2-propenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
4-(1,1,4-Trioxo-(1,2,5)thiadiazolidin-2-yl)benzoic acid methyl ester
729600-47-97 729600-48-09-729600-49-1P
729600-50-4P 729600-51-5P 729600-52-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(prepn. of sulfahydantoins as phosphate isosteres for use as protein

phosphatase inhibitors in treatment of cancer and autoimmune disorders)

disorders)
RN 612527-99-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
methyl ester (9CI) (CA INDEX NAME)

RN 612530-69-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 729600-44-6 HCAPLUS CN Benzoic acid, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl ester (9C1) (CA NDEX NAME)

L4 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 729600-50-4 HCAPLUS CN Benzamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9C1) (CA INDEX NAME)

RN 729600-51-5 HCAPLUS
CN Benzamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N(phenylmethyl)- {9CI} (CA INDEX NAME)

RN 729600-52-6 HCAPLUS
CN Benzamide, N-butyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI)
(CA INDEX NAME)

ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Sulfamides, such as I, were prepared for use as anticancer agents which

by modulating the activation states of abl or bcr-abl α -kinase proteins. Thus, 4-H02CC6H4CH2NHSO2NHCOR [R = pyrrolidino], prepared from 4-Me02CC6H4CH2NH2 and pyrrolidine, was treated with the pyrimidinylaminoaniline fragment to give I, which showed 10% inhibition

non-phosphorylated abl kinase at 10µM.
726192-44-5P 726192-45-6P 726192-60-5P
726192-61-6P
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of sulfamides as anti-cancer agents)
726192-44-5 HCAPLUS
Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-methyl]-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino)phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 23 Jul 2004
ACCESSION NUMBER: 2004:589375 HCAPLUS
141:140459
TITLE: INVENTOR(S): Proparation of sulfamides as anti-cancer agents
Flynn, Daniel L.: Petrillo, Peter A.
POT Int. Appl., 168 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT:

	PA?	TENT	NO.			KIN		DATE				LICAT					ATE	
		2004				A2						2003-					0031	
1	WO	2004																
		W:										, BG,						
												, EE,						
												, KG,						
												, MW,						
												, SL,	TJ,	TM,	TN,	TR,	TT,	ΤZ,
								VN,										
		RW:										, SZ,						
												, BG,						
												, MC,						
			TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GA,	GN	, GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,
TG																_		
		2004				A1		2004	0902		US	2003- 2003-	7465	45		2	0031	224
		2004		95		Al												
		2511				A1						2003-						
		2003		39		A1		2004	0729		ΑU	2003- 2003-	3036	39		2	0031	226
	ΕP	1590				A2												
		R:										, IT,						PT,
												, TR,						
		2003		63		A		2005	1206		BH	2003- 2003-	1,86	3		-	0031	226
		1756				Α.		2006	0405		CN	2003-	0011	0049		-	0031	220
	CN	1791	596			Α.		2006	0621		CN	2003-	8011	22			0031	226
	JP.	2006	219/	65		Т		2006	0831		JP	2005- 2002-	4777	23			0031	220
PRIOR	1T:	Y APP	TW.	INFO	. :						US	2002-	43/3	042		P 2	0021	231
											US	2002-	4374	03P		P 2	0021	231
											ŲS	2002-	4374	15P		P 2	0021	231
											US	2002-	4374	87P		P 2	0021	231
											US	2003-	4638	04P		P 2	0030	41B
											US	2003-	7465	45		A 2	0031	224
											US	2003-	7466	07		A 2	0031	224
											wo	2003-	US 4 1	425		W 2	0031	226

OTHER SOURCE(S):

MARPAT 141:140459

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

726192-45-6 HCAPLUS Benzamide, 4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-{4-methyl-3-(14-phenyl-2-pyrimidinyl)mmino|phenyl|- (9C1) (CA INDEX NAME)

726192-60-5 HCAPLUS
Benzamide, 4-[(3,3-dimethyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-methyl-3-(2-pyrimidinylamino)phenyl]- (9CI) (CA INDEX NAME)

ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-00-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-(9C1) (CA INDEX NAME)

L4 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

612527-99-8P 612528-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfamides as anti-cancer agents)
612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Encered STN: 18 Jun 2004
ACCESSION NUMBER: 2004:493593 HCAPLUS
DOCUMENT NUMBER: 141:54348
TITLE: Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as inhibitors of protein tyrosine phosphatase lB
INVENTOR(5): Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin
APATENT ASSIGNEE(5): Astrazeneca AB, Swed.; Astrazeneca UK Limited
PCT Int. Appl., 48 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATEN	T NO				KIN	D	DATE			APPL	ICAT	ION :	NO.		D	ATE	
						-											
WO 20	0405	06	46		A1		2004	0617		WO 2	003-	GB51	20		21	0031	126
W	: A	Ε,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
							DK,										
	G	Н,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,
	L	R,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MΧ,	ΜZ,	ΝI,	NO,	ΝZ,
	0	м,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,
	T	N,	TR,	TT,	TZ,	UA,	ŰĠ,	US,	UZ,	νc,	VN,	YU,	ZA,	ZM,	ZW		
R	W: B	W,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	ΤZ,	UG,	ZM,	ZW,	AM,	AZ,
	В	Υ,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,
	E	s,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	sĸ,
	Ť	R,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,
	-	•••	,	_,	,		/		-7.					,			

AU 2003302626 PRIORITY APPLN. INFO.: 20040623 WO 2003-GB5120 W 20031126

OTHER SOURCE(S): MARPAT 141:54348

Title compds. I [wherein Rl = H, (halogeno)alkyl, (hydroxy)alkoxy, alkylamino, etc.; R2 = H, (halogeno)alkyl, halogeno, alkoxy; R3 = alkylamido or (un)substituted alkyl; R4 = H, alkyl, (hetero)aryl; R5 = H or alkyl; and pharmaceutically acceptable salts thereof] were prepared as inhibitors of protein tyrosine phosphatase 1B (PTB1B). For example, 5-[4-(accetamidomethyl)-2-methoxyphenyl]-1,2,5-thiadiazolidin-1-one 1,1-dioxide (II) was given in multi-step synthesis starting from

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
3-methoxy-4-nitrobenzyl alc. II showed inhibition of human PTBIB with
ICSO value of 44pM. Thus, I and their pharmaceutical compns. are
useful as inhibitors of protein tyrosine phosphatase IB for the treatment
of diabetes medilitus.
052256-50-4P 705256-58-8P 705256-78-70705256-8P-705256-86-79-705256-87-2P
705256-86-70 705256-87-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of 5-phenyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide

(Uses)
(preparation of 5-phenyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide
derivs. as
inhibitors of protein tyrosine phosphatase 1B)
RN 705256-50-4 HCAPLUS
CN Actamide, N-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-54-8 HCAPLUS
Benzeneacetonitrile, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(9C1) (CA INDEX NAME)

705256-55-9 MCAPLUS Acetamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-3-methoxyphenyl|methyl]- (9CI) (CA INDEX NAME)

ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 705256-72-0 HCAPLUS Benzenepentanamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- {9CI} (CA INDEX NAME)

Ph- (CH₂)₄-C

705256-78-6 HCAPLUS Acetamide, N-(14-(3-methyl-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl]- (9CI) (CA INDEX NAME)

705256-92-2 HCAPLUS Acetamide, N-(2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT:

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

705256-61-7 HCAPLUS Butanamide, N-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl)- (9CI) (CA INDEX NAME)

705256-67-3 HCAPLUS Benzenepropanaide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-methyl- (9C1) (CA INDEX NAME)

L4 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 21 May 2004 ACCESSION NUMBER: 2004:412929 HCAPLUS DOCUMENT NUMBER: 140:423678 Preparation of 5-(substituted beneather)

phenyl) thiadiazolidin-3-

ones as inhibitors of protein tyrosine phosphatase 1B Birch, Alan Martin; Kenny, Peter Wedderburn; Morley, Andrew David; Russell, Daniel John; Toader, Dorin Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 89 pp. CODEN: PIXXD2

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. 								APPLICATION NO.						DATE			
								0521	WO 2003-GB4721							20031103	
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		co,	CR,	CU,	cz,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	GΕ,
		GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	K₽,	KR,	ΚZ,	LC,	LK,
		LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MΧ,	ΜZ,	NI,	NO,	NZ,
		OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	5Κ,	SL,	SΥ,	ТJ,	TM,
		TN,	TR,	TT,	TZ,	UA,	UG,	US,	υz,	VC,	VN,	YU,	ZA,	ZM,	zw		
	RW:	BW,	GH,	GM,	KE,	LS,	MW.	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,
		BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,
		ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	IT,	LU,	MÇ,	NL,	ΡŤ,	RO,	SE,	SI,	SK,
		TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝĒ,	SN,	TD,

AU 2003278392 PRIORITY APPLN. INFO.: WO 2003-GB4721 W 20031103

OTHER SOURCE(S):

MARPAT 140:423678

AB The title compds. (I) or pharmaceutically acceptable salts thereof [Rl = H, halo, Cl-6 alkyl, Cl-6 alkoxy, Cl-6 alkylthio, halo-Cl-6 alkyl, halo-Cl-6 alkoxy, halo-Cl-6 alkoxy, dihydroxy-Cl-6 alkoxy, dihydroxy-Cl-6

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CO2H

692764-76-4P 692764-77-5P 692764-78-6P
692764-79-P 692764-80-0P 692764-81-1P
692764-82-P 692764-83-3P 692764-81-1P
692764-85-SP 692764-86-6P 692764-87-7P
692764-88-BP 692764-86-6P 692764-90-2P
692764-91-3P 692764-99-P 692764-90-2P
692764-91-3P 692764-95-7P 692764-90-2P
692764-91-3P 692764-95-7P 692764-90-4P
692765-00-PP 692765-01-8P 692764-99-1P
692765-00-PP 692765-01-8P 692765-02-9P
692765-01-3P 692765-01-4P 692765-02-9P
692765-10-9P 692765-11-0P 692765-02-9P
692765-10-9P 692765-14-3P 692765-12-1P
692765-13-2P 692765-14-3P 692765-12-1P
692765-13-2P 692765-14-3P 692765-12-1P
692765-20-1P 692765-13-4P 692765-12-1P
692765-20-1P 692765-13-4P 692765-12-4P
692765-20-3P 692765-13-4P 692765-23-4P
692765-32-4P 692765-31-3P 692765-31-4P
692765-32-8P 692765-31-8P 692765-31-4P
692765-33-8P 692765-31-8P 692765-31-4P
692765-33-8P 692765-31-8P 692765-31-4P
692765-34-1P 692765-31-8P 692765-31-4P
692765-30-1P 692765-31-4P 692765-40-5P
692765-30-1P 692765-31-4P 692765-50-4P
692765-30-1P 692765-31-4P 692765-50-4P
692765-30-1P 692765-31-4P 692765-50-5P
692765-30-1P 692765-31-4P 692765-50-5P
692765-30-1P 692765-61-8P 692765-61-0P
692765-30-1P 692765-61-8P 692765-61-0P
692765-30-4P 692765-60-9P 69

(USES)
(preparation of phenylthiadiazolidinones as inhibitors of protein tyrosine

phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
692764-76-4 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 5-(4'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) alkoxy, C1-6 alkoxy-C1-6 alkoxy, aryloxy, aryl-C1-6 alkoxy, aryloxy-C1-6 alkoxy, aryloxy-C1-6 alkoxy, heteroaryloxy, heteroaryloxy-C1-6 alkoxy, C1-6 alkoxy, C1-6 alkylthio, C1-6 alkylthio-C1-6 alkoxy, C1-6 alkylsulfinyl-C1-6 alkoxy, C1-6 alkylsulfonyl-C1-6 alkoxy, aryl-C1-6 alkylthio, etc., R2 - H, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio, etc., C1-6 alkylthio, C1-6

they are attached form a 5-7 membered carbocyclic or heterocyclic ring;

and R4 are selected such that (i) R3 = hýdrogen, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylthio or halo and R4 = aryl, biaryl, heteroaryl, C2-6 alkynyl, C3-7 cycloalkyl, arylcarbonyl, heteroarylcarbonyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl, or (ii) R4 = H, C1-6 alkyl, C1-6 alkoy, C1-6 alkylthio, or halo and R3 = aryl, biaryl, heteroaryl, C2-6 alkynyl, C3-7 cycloalkyl, arylcarbonyl, heteroarylcarbonyl, aryl-C2-6 alkoyl arylcarbonyl arylcarbon

alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H, C1-6

aryl-C2-6
alkenyl, aryl-C2-6 alkynyl or heteroaryl-C2-6 alkenyl; R5 = H. C1-6
alkyl.
C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkyl, halo; R6 = H, C1-6 alkyl;
wherein any aryl, biaryl or heteroaryl group is optionally substituted]
are prepd. These compds are useful as inhibitors of protein tyrosine
phosphatase PTP1B for the treatment of diabetes mellitus. Thus,
4-tolylboronic acid was coupled with 5-(4-bromophenyl)-1,2,5thiadiazolidin-3-one in the presence of
tetrakis(triphenylphosphine)pallad
ium(0) [Pd(PPh3)4] and cesium carbonate in a mixt. of DMF, DME, EtOH, and
H2O at 170° for 600 s to give 5-(4'-Methyl-1,1'-biphenyl-4-yl)1,2,5-thiadiazolidin-3-one 1,1-dioxide.
IT 692765-08-5P 692765-17-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of phenylthiadiazolidinones as inhibitors of protein
tyrosine
phosphatase 1B (PTP1B) for treatment of diabetes mellitus)

phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
692765-08-5 HCAPIUS
[1,1'-Biphenyl]-4-carboxylic acid, 3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'-methoxy- (9CI) (CA INDEX NAME)

692765-17-6 HCAPLUS
[1,1'-Biphenyl]-3-carboxylic acid, 3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-4'-methoxy- (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692764-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3'-nitro[1,1'-biphenyl]-4-yl)-, (9CI) (CA INDEX NAME)

v.z.vo='10=0 m.A.P.U.S 1,2,5=Thiadiazolidin=3-one, 5-(3',5'-dichloro(1,1'-biphenyl)-4-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-79-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

692764-80-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-4-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin 692764-83-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3'-methyl(1,1'-biphenyl)-3-yl)-,1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

692764-84-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[4'-(methylthio)[1,1'-biphenyl]-3-yl]-,
1,-dioxide (9CI) (CA INDEX NAME)

692764-85-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(4'-methyl{1,1'-biphenyl}-3-yl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

692764-86-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2'-methyl[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692764-81-1 HCAPLUS Acetamide, N-[4'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-3-yl]- (9CI) (CA INDEX NAME)

692764-82-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692764-87-7 HCAPLUS Acetamide, N-(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)[1,1'-biphenyl]-3-yl]- (9CI) (CA INDEX NAME)

692764-88-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[3-(2-benzofuranyl)phenyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

692764-89-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1'-biphenyl]-3-yl)-.
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Meo N

RN 692764-90-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[3-(5-oxezolyl)phenyl]-, 1,1-dioxide (9CI) (CA INDEX NARE)

RN 692764-91-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-cyclohexylphenyl)-, 1,1-dioxide (9CI)
(CA INDEX NAME)

H N

RN 692764-92-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3-benzoylphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO F

RN 692764-96-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4,4'-dimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

Meo OMe

RN 692764-97-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-4'-phenoxy[1,1'-blpheny1]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

Meo OPh

RN 692764-98-0 HCAPLUS CN [1,1'-Biphenyl]-3-carbonitrile, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9C1) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Ph-C

RN 692764-93-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-4-yl-, 1,1-dioxide (9CI)
(CA INDEX NAME)

H N S

RN 692764-94-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[1,1'-biphenyl]-3-yl-, 1,1-dioxide (9CI) (CA INDEX NAME)

H

RN 692764-95-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-fluoro-4-methoxy(1,1'-biphenyl)-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

H S O

RN 692764-99-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-nitro[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

MeO No

RN 692765-00-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{3',4-dimethoxy[1,1'-biphenyl]-3-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

MeO MeO

RN 692765-01-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-hydroxy-4-methoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-02-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',4,4'-trimethoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-03-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-04-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{5-(1,3-benzodioxol-5-yl)-2-methoxyphenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-09-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1E)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-10-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[2-naphthalenyl]phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4'-(hydroxymethyl)-4-methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-05-2 HCAPLUS
N Acetamide, N-{3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy(1,1'-bipheny1)-3-y1|- (9CI) (CA INDEX NAME)

RN 692765-06-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy-3'-methyl[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-07-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{3'-acetyl-4-methoxy{1,1'-biphenyl}-3-yl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-12-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-,1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-13-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(phenylmethoxy)[1,1'-biphenyl]-3-yl]-,1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-14-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(phonylmethoxy)[1,1'-biphenyl]-3-yl]-,1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-15-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[(1Z)-2-phenylethenyl]phenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 692765-16-5 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-[4'-[(1,1-dimethylethoxy)methyl]-4methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-18-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-4'-(methoxymethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide [9CI] (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-22-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3',5'-difluoro-4-methoxy[1,1'-biphenyl]-3yl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-23-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5'-fluoro-2',4-dimethoxy[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-24-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methoxy[1,1':3',1''-terphenyl]-3-yl)-, 1,1-dioxide (9C1) (CA INDEX NAME) L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-19-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methowy-3'-(methylthio)[1,1'-biphenyl]-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-20-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-acetyl-4-methoxy[1,1'-biphenyl]-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-21-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy(1,1'-biphenyl)-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 692765-25-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2'-fluoro-4-methoxy{1,1'-biphenyl}-3-yl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{4-methoxy-4'-(methylthio){1,1'-biphenyl}-3yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-27-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{4'-(1,1-dimethylethyl)-4-methoxy[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

MeO Bu-t

RN 692765-28-9 HCAPLUS
CN 1,2,5-Thladiazolidin-3-one, 5-(4-methoxy[1,1':4',1''-terphenyl]-3-yl)-,
1,1-dioxide (9C1) (CA INDEX NAME)

MeO Ph

RN 692765-29-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-chloro-4'-fluoro-4-methoxy{1,1'-biphenyl|3-y-1|}-1,1-dioxide (9CI) (CA INDEX NAME)

MeO C1

RN 692765-30-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-fluoro-4-methoxy[1,1':4',1''-terphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

 $\begin{array}{c} \text{H} & \text{O} \\ \text{N} & \text{S} \\ \text{O} \\ \text{N} & \text{CH} = \text{CH}_2 \\ \end{array}$

RN 692765-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(2-furany1)-2-methoxypheny1]-,
1,1-dioxide (9CI) (CA INDEX NAME)

° S NH

RN 692765-35-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-benzo[b]thien-2-yl-2-methoxyphenyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

OME NH

RN 692765-36-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-[2-benzofuranyl]-2-methoxyphenyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

OME N S NH

RN 692765-37-0 HCAPLUS .
CN 1,2,5-Thiadiazolidin-3-one, 5-(4'-acetyl-4-methoxy(1,1'-biphenyl)-3-yl)-,

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Meo Ph

RN 692765-31-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-methoxy-3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Meo CF3

RN 692765-32-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-{(1E)-2-(4-chlorophenyl)ethenyl]-2-methoxyphenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

He O

RN 692765-33-6 HCAPLUS (N 1,2,5-Thiadiazolidin-3-one,5-(4'-ethenyl-4-methoxy[1,1'-biphenyl]-3-yl)-,1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 1,1-dioxide (9CI) (CA INDEX NAME)

Meo Ac

RN 692765-38-1 HCAPLUS CN [1,1'-Biphenyl]-3-carboxamide, 3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9C1) (CA INDEX NAME)

MeO C-NH2

RN 692765-39-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(1H-pyrazol-4-yl)phenyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

HN S NI

RN 692765-40-5 HCAPLUS
CN Pyrrolidine, 1-[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy(1,1'-bipheny1)-4-y1)carbony1|- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-41-6 HCAPLUS CN [1,1'-Biphenyl]-4-propanoic acid, 3'-(1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-42-7 HCAPLUS
CN Carbamic acid, [(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA
INDEX NAME)

RN 692765-43-8 HCAPLUS
CN [1,1'-Biphenyl]-3-carboxamide,
3'-(1,1-dioxido-4-oxo-1,2,5-thladiazolidin2-yl)-4'-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 3-yl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-47-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[4-pyridinyl]phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-48-3 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 5-(4'-hydroxy-4-methoxy[1,1'-biphenyl}-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-49-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[5-(1H-indol-6-yl)-2-methoxyphenyl)-,
1,1-dioxide (SCI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-44-9 HCAPLUS CN [1,1"-Biphenyl]-4-carboxamide, N-cyclohexyl-3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy- (9CI) (CA INDEX NAME)

RN 692765-45-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(3'-amino-4-methoxy[1,1'-biphenyl]-3-y1)-,
1,1-dioxide, monchydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 692765-46-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[4'-(dimethylamino)-4-methoxy{1,1'-biphenyl}-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 692765-50-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(2-thienyl)phenyl}-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-51-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(2-methoxy-5-(phenylethynyl)phenyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 692765-52-9 HCAPLUS (1.2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-(3-phenyl-1-propynyl)phenyl]-, 1,1-dioxide (901) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 6927(65-53-0 KCAPLUS 1,2,5-Thiadiezolidin-3-one, 5-(5-ethynyl-2-methoxyphenyl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 692765-54-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-methyl[1,1'-biphenyl]-3-yl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-56-3 RCAPLUS
Benzoic acid, 2-[2-[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA RN CN

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-60-9 HCAPLUS
Benzoic acid, 2-{2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-biphenyl]-4-y1)ethoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

692765-61-0 HCAPLUS

Benzoic acid, 2-[2-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-4-yl]ethoxy]-6-hydroxy-, methyl ester (9CI) (CA

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN INDEX NAME) (Continued)

692765-57-4 HCAPLUS
Benzoic acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]methoxyl-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-58-5 HCAPLUS
Benzolc acid, 2-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-4-y1]methoxy[-6-hydroxy- (9CI) (CA INDEX NAME)

692765-59-6 HCAPLUS
Benzoic acid, 2-[{3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-4'-methoxy{1,1'-biphenyl}-4-y1]methoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

692765-63-2 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]propoxy]-6-hydroxy-, methyl ester (9CI) (CA
INDEX NAME)

692765-64-3 HCAPLUS
Benzoic acid, 2-[3-[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-4-yl)propoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

692765-65-4 HCAPLUS
Benzoic acid, 2-[3-[3'-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'-methoxy[1,1'-bipheny1]-4-y1]propoxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-66-5 HCAPLUS
Benzoic acid, 2-[(3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-methoxy[1,1'-biphenyl]-3-yl]methoxy]-6-hydroxy- (9CI) (CA INDEX NAME)

692765-67-6 HCAPLUS
{1,1'-Biphenyl]-3-carboxamide,
{1,1-dioxido-4-oxo-1,2,5-thiadiarolidin2-yl)-4'-methoxy-N-{2-phenoxyethyl}- (9CI) (CA INDEX NAME)

NH-CH2-CH2-OPh

RN 692765-68-7 HCAPLUS
CN Benzoic acid,
2-[2-[[[3'-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'methoxy[1,1'-bipheny1]-3-y1]carbony1]amino]ethoxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzoic acid,
2-[6-[[3]-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4'mentoxy[1,1'-biphenyl]-3-yl]carbonyl]amino]hexyl]oxy]-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME)

0- (CH2) 6-NH

692765-72-3 HCAPLUS

RN 692765-73-4 HCAPLUS
CN Benzoic acid,
[3-([3-([3]-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-4-yl|carbonyl|amino|propoxy|-6-hydroxy-, methyl
ester (9CI) (CA INDEX NAME) 692765-73-4 HCAPLUS

RN 692765-74-5 HCAPLUS CN Benzoic acid, 2-{[5-[[3'-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'-

L4 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 692765-69-8 HCAPLUS
CN Benzolc acid,
2-[3-[[3]-([3]-(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4'methoxy[1,1'-biphenyl]-3-yl]carbonyl]amino[propoxy]-6-hydroxy-, methyl
ester (9C1) (CA INDEX NAME)

RN 692765-70-1 KCAPLUS
CN Benzoic acid,
2-[[5-[[3]" -[1, 1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-4"methoxy[1,1"-biphenyl]-3-y1]carbonyl)amino]pentyl]oxy]-6-hydroxy-, methyl
ester (9C1) (CA INDEX NAME)

692765-71-2 HCAPLUS

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) methoxy[1,1'-biphenyl]-4-yl[carbonyl]amino[pentyl]oxy]-6-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

IT 692765-79-0P 692765-80-3P 692765-84-7P
692765-85-8P 692765-86-9P 692766-02-2P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylthiadiazolidinones as inhibitors of protein tyrosine
phosphatase 1B (PTP1B) for treatment of diabetes mellitus)
RN 692765-79-0 MCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(4-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

692765-80-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(3-bromophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

692765-84-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(5-bromo-2-methoxyphenyl)-, 1,1-dioxide (9C1) (CA NNDEX NAME)

692765-85-8 HCAPLUS Boronic acid, [3-[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)

692765-86-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[2-methoxy-5-[4,4,5,5-tetramethyl-1,3,2-

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 10 OCC 2003 ACCESSION NUMBER: 2003:796679 HCAPLUS DOCUMENT NUMBER: 139:307766

TITLE: Preparation of substituted 1,1-dioxo-1,2,5-thiazolidine-3-ones as protein tyrosine phosphatase

INVENTOR(S):

and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis Coppola, Gary Mark; Davies, John William; Jewell, Charles Francis, Jr.; Li, Yu-Chin; Wareing, James Richard; Sperbeck, Donald Mark; Stams, Travis Mathew; Topiol, Sidney Wolf; Vlattas, Isidoros Novartis A.-G., Switz:, Novartis Pharma G.m.b.H. PCT Int. Appl., 148 pp. CODEN: PIXXD2
Patent
English

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT	NO.			KIN	0	DATE		1	APPL	ICAT	ION	NO.		D	ATE	
								09 WO 2003-EP3466									
											BG;						
											EE,						
		HD,	HII	TD.	T.L.	IN.	TS.	JP.	KE.	KG.	KP,	KR.	KZ.	LC.	LK.	LT.	LU
		T.V	MA.	MD.	MK.	MN.	MX.	NT.	NO.	NZ.	OM,	PH.	PL.	PT.	RO.	RU.	sc
											US,						
	RW:	DM.	A7	BY.	KG,	K 7	MD	RII.	TJ.	TM.	AT.	BE.	BG.	CH.	CY.	cz.	DE.
	A	DK.	FF.	F.S.	PT.	FR	GB,	GR.	HU.	IE.	IT,	LU.	MC.	NL.	PT.	RO.	SE
		S.T.	SK	TD													
42	2480	562	J.,	***	A1		2003	1009		CA 2	003-	2480	562		2	0030	402
AII	2003224030			A1 20031013			AU 2003-224030					20030402					
115	2004023974			A1 20040205			CA 2003-2480562 AU 2003-224030 US 2003-405728 CS 2003-720412						20030402				
ED	1492	780			A1		2005	0105	S	P 0 - 0	003=	7204	12		2	0030	402
	p.	TA.	BE.	CH.	DE.	DK.	ES.	FR.	GB.	GR.	IT,	LI.	LU.	NL.	SE.	MC.	PT
		TP	e t	1.0	T.V	FT	P.O	MK	CY	AT.	TR.	BG.	CZ.	EE.	HU.	SK	
BR	2003 2005 1646 2005 2004	0089	74	,	Α,	,	2005	0215		BR 2	003-	8974			2	0030	402
US	2005	0905	02		Al		2005	0428	-	0S 2	003-	5100	26		2	0030	402
CN	1646	508			A		2005	0727	•	CN 2	003-	8078	87		2	0030	402
JP	2005	5355	68		т		2005	1124		JP 2	003-	5803	08		2	0030	402
NO	2004	0047	45		Ā		2004	1214		NO 2	004-	4745			2	0041	102
RIT	APP	LN.	INFO	.:	•••				,	US 2	002~	3697	79P		P 2	0020	403
										US 2	002-	3699	30P		P 2	0020	403
									,	WO 2	003-	EP34	66		w 2	0030	402

OTHER SOURCE(S): MARPAT 139:307766 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) dioxaborolan-2-yl)phenyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 692766-02-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-(5-iodo-2-methoxyphenyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

$$\begin{array}{c|c}
0 & 1 & X \\
0 & 1 & X \\
0 & 1 & 2 \\
0 & 2 & 2 \\
\end{array}$$

$$\begin{array}{c|c}
1 & X & Y \\
2 & 2 & 2 \\
\end{array}$$

$$\begin{array}{c|c}
1 & 1 & 2 & 2 \\
\end{array}$$

$$\begin{array}{c|c}
1 & 2 & 2 & 2 \\
\end{array}$$

Substituted thiarolidinetriones I [L1 = L2 = single bond; 01 = single bond, H, (un)substituted alkyl, cycloalkyl, or aminocarbonyl, carboxy, R10C(:0), R10C(:0), R10G(:0), R20S(:0)q, Q2 = 0, S, R3N, R, R2 = (un)substituted alkyl, alkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, or aralkylthio, amino, halogen, nitro, carboxy, trifluoromethyl, etc.; R1 = (un)substituted alkyl, alkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkoxy, aralkoxy, aralkyl, alkynyl, heteroalkyl, aryl, heteroaryl, aralkyl, alkyl; R10 = (un)substituted alkyl, alkoxycarbonyl, aryl, heteroaryl, aralkyl, heteroaryloxycarbonyl, carbanyl, or sulfonyl; X, Y = (H, N, O, S, R14N; Z = (un)substituted alkyl, alkoxyalkyl, alkylthioalkyl, alkylaminoalkyl; Z1, Z2, Z3 = CH, N, (1:0), CR, CR2; R1 and R2 can form an (un)substituted 5 -, or 6-membered aromatic or heteroarom. ring; R1 and L1 can form an (un)substituted 5 -, or

6- or
7-membered ring interrupted by nitrogen, oxygen or sulfur atoms] such as
II are prepared as inhibitors of protein tyrosine phosphatase 1b and

protein tyrosine phosphatase for overcoming insulin resistance and modulating glucose levels in the treatment or prevention of metabol diseases, such as diabetes, or atherosclerosis. II is prepared by

treatment of Et bromoacetate with 1-naphthalenemethanamine, N-sulfamoylation with sulfamoyl chloride, and base-mediated cyclocondensation. No biol data

provided.
612530-89-8P 612530-90-2P 612530-92-4P 612530-93-5P 612530-94-6P 612530-99-4P 612530-99-4P 612530-99-1P 612530-99-1P 612530-99-1P 612531-03-97 612531-73-97 612531-7

ANSWER 15 OF 33 RCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612531-80-3P 612534-94-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate; prepn. of thiazolidinetriones as protein tyrosine
phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to
mitigate insulin resistance in the treatment of diabetes or
atherosclerosis)
612530-89-9 RCAPLUS
Carbanic acid, [4-[5-((2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl]methyl]phenyl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612530-90-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-{(2,4-dimethoxyphemyl]methyl}-5-{(1-ethyl-2methyl-1H-benzimidazol-5-yl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued)

RN 612530-92-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl)-5-[(4-methoxy-7-quinolinyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612530-93-5 HCAPLUS
CN Benroic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl}-, [4-(methylthio)phenyl]methyl ester (9CI)
(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612530-94-6 HCAPLUS
CN Benzoic acid,
4-[5-[2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5thiadiarolidin-2-yl]methyl]-, [4-(methylsulfonyl)phenyl]methyl ester

(9CI)

(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

612530-95-7 HCAPLUS
1,2,3-Thiadiarolidin-3-one, 5-[[4-(bromomethyl)phenyl]methyl]-2-[(2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-96-8 HCAPLUS
Acetic acid, [[4-[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612530-99-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-iodophenyl)methyl}-2-{(4-methoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A .

PAGE 2-A

612530-98-0 HCAPLUS Acetic acid, [[4-[[5,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612531-00-7 HCAPLUS L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-3-[{5-{(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-01-8 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-3-[{5-[(4-

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-02-9 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[(4-methoxyphenyl)methyl)-1,1-dioxido-4-oxo1,2,5-thiadiazolidin-2-yl)methylphenylmethyl)-2-oxo-2(pentylamino)ethyl}-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-03-0 HCAPLUS
Benzenepropanamide, \(\alpha \) = mino-3-[[5-[(4-methoxyphenyl)methyl]-1, l-dioxido-4-oxo-1, 2, 5-thiadiazolidin-2-yl]methyl]-N-pentyl-, (\(\alpha \) S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-13-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl)-5-[[4-[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

PÂGE 1-A

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-05-2 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-[[5-[(4-

methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-10-9 HCAPLUS
CN Benzaldehyde,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612531-22-3 HCAPLUS
Carbamic acid, [[4-[[5-[(2,4-dimethoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]-, 1,1-dimethylethyl ester (SCI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

612531-23-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-2-[{2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-24-5 HCAPLUS
CN Carbamic acid,
[2-{[{4-{[5-{(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-chiadiazoliddin-2-yl]methyl]phenyl]methyl]amino]-2-oxoethyl}-,
1,1-dimethylethyl ester (9CI) {CA INDEX NAME}

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612531-31-4 HCAPLUS
CN Benzoic acid,
4-[[5-[(2,4-dimethoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612531-30-3 HCAPLUS
CN Benzoic acid,
4-[[5-{(2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5thiadiazolidin-2-yl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-32-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, [4-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612531-34-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[(2,4-dimethoxyphenyl)methyl]-5-(2,4-dimitrophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-35-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-2-[(2,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-63-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-2-(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612531-64-3 HCAPLUS
CN L-Phenylalanine, N-{(1,1-dimethylethoxy)carbonyl}-4-{5-{(4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-36-9 HCAPLUS
CN Benzoic acid, 3-{5-{(2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, methyl ester (9CI) (CA INDEX NAME)

RN 612531-61-0 HCAPLUS
CN 1H-1,4-Benzodiazepine-2,5-dione, 3-[{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-(phenylmethoxy)phenyl]methyl]-3,4-dihydro- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612531-65-4 HCAPLUS
CN D-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612531-66-5 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612531-67-6 HCAPLUS
CN Carbamic acid,
[(1S)-1-[[4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-chiadiacolidin-2-yllphenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-68-7 HCAPLUS Benzenepropanamide, α -amino-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-69-8 HCAPLUS L-Phenylalanyl-4-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl (9C1) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612531-72-3 HCAPLUS
L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-[(4-methoxyphenyl)methyl]1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-73-4 HCAPLUS
L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-[4-[2-(1,1-dimeth)]-4-[5-[(4-methoxy)-2-oxethyl]]-4-[5-[(4-methoxyphenyl]]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

612531-70-1 HCAPLUS L-Phenylalanine, 4-[5-{(4-methoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-71-2 HCAPLUS L-Phenylalanine, N-acetyl-L-phenylalanyl-4-[5-{{4-methoxyphenyl}methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-75-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(3-iodophenyl)-, 1,1-dioxide (9CI) (CA
INDEX NAME)

RN 612531-76-7 HCAPLUS CN 1,2,5-Thiadia*colidin-3-one, 5-(3-iodopheny1)-2-[(4-methoxypheny1)methy1]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612531-77-8 HCAPLUS
L-Phenylalanine, N-{[1,1-dimethylethoxy)carbonyl]-3-[5-[{4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612531-78-9 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl}-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]- (9CI)(CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612534-94-8 HCAPLUS L-Phenylalanianide, N-acetyl-L-phenylalanyl-3-[5-[(4-methoxyphenyl]methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl- (9CI)- (CA INDEX NAME)

Absolute stereochemistry.

612527-93-2P 612530-46-8P 612530-49-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (invention compound; preparation of thiazolidinetriones as protein sine

sine
phosphatase lb and T-cell protein tyrosine phosphatase inhibitors to
mitigate insulin resistance in the treatment of diabetes or
atherosclerosis]
612527-93-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-aminophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612531-79-0 HCAPLUS
CN Carbamic acid,
[(1S)-1-[(3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo1,2,5-chiadiazolidin-2-yllphenyl]methyl]-2-oxo-2-(pentylamino)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

(Continued)

Absolute stereochemistry.

612531-80-3 HCAPLUS Benzenepropanamide, \(\alpha\)-amino-3-[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]-N-pentyl-, (\(\alpha\)5) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-46-8 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-, methyl
ester (9CI) (CA INDEX NAME)

612530-49-1 HCAPLUS
Benzeneacetic acid, 2-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-, methyl ester (9CI) (CA INDEX NAME)

612527-84-1P 612527-85-2P 612527-86-3P 612527-87-4P 612527-89-5P 612527-89-6P 612527-89-6P 612527-89-5P 612527-91-0P 612527-91-0P 612527-91-0P 612527-91-0P 612527-91-0P 612527-97-6P 612527-91-0P 612528-00-4P 612528-01-5P 612528-00-3P 612528-07-3P 612528-07-3P 612528-07-3P 612528-07-3P 612528-07-3P 612528-13-0P 61252

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 612528-17-3P 612528-18-4P 612528-19-5P 612528-21-9P 612528-22-0P 612528-23-1P 612528-23-3-3P 612528-33-3P 612528-33-3P 612528-33-3P 612528-33-3P 612528-33-3P 612528-33-3P 612528-33-3P 612528-33-3P 612528-42-P 612528-41-3P 612528-31-3P 612528-41-3P 612528-41-3P 612528-42-4P 612528-41-3P 612528-41-3P 612528-42-4P 612528-41-3P 612528-41-3P 612528-45-7P 612528-41-3P 612528-45-7P 612528-52-6P 612528-52-6P 612528-53-3P 612528-53-3P 612528-53-3P 612528-53-3P 612528-60-6P 612528-61-7P 612528-61-P 612529-10-P 612529-10-P 612529-11-P 6 (Continued)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
612530-08-2P 612530-09-3P 612530-10-6P
612530-11-7P 612530-12-8P 612530-13-9P
612530-16-2P 612530-12-8P 612530-21-9P
612530-19-5P 612530-20-8P 612530-21-9P
612530-22-0P 612530-23-1P 612530-28-6P
612530-22-7P 612530-31-3P 612530-28-6P
612530-22-7P 612530-31-3P 612530-28-6P
612530-35-5P 612530-31-3P 612530-31-1P
612530-35-5P 612530-31-3P 612530-37-7P
612530-41-3P 612530-31-6P 612530-37-7P
612530-41-3P 612530-42-4P 612530-47-9P
612530-48-0P 612530-65-7P 612530-47-9P
612530-48-0P 612530-50-4P 612530-47-9P
61250-48-0P 612530-50-4P 612530-47-9P
612530-48-0P 612530-47-9P
61250-48-0P 612530-47-9P
612530-48-0P 612530-47-4P
612530-48-0P 612530-47-4P
612530-48-0P 612530-47-4P
612530-48-0P 612530-47-

612527-85-2 HCAPLUS
Acetamide, N-[[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}pheny1)methy1)- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-86-3 HCAPLUS
Carbmic acid, [3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y)]methyl]phenyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA (CA INDEX NAME)

612527-87-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612527-88-5 HCAPLUS Acetamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN y1)methy1)pheny1}methy1]- (9CI) (CA INDEX NAME)

612527-89-6 HCAPLUS
Carbamic acid, [[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y]]methyl]henyl]methyl]-, 1,1-dimethylethyl ester [9C1] (CA INDEX NAME)

612527-90-9 HCAPLUS
Benzenepropanamide, N-[[4-[[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]- [9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-91-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{(3-iodophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-92-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-nitrophenyl)methyl]-, 1,1-dioxide (9CI)
(CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)

RN 612527-98-7 HCAPLUS CN Urea, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]-N'-propyl- (9CI) (CA INDEX NAME)

612527-99-8 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612527-94-3 HCAPLUS
Acetamide, N-[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

612527-96-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-{{4-aminophenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

612527-97-6 HCAPLUS
Butanamide, N-[3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl}- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-00-4 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-(9C1) (CA_INDEX_NAME)

612528-01-5 HCAPLUS
Benzoic acid, 2-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-(9CI) (CA INDEX NAME)

612528-02-6 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methylphenyl)methyl]-, 1,1-dioxide
(9CI)
(CA INDEX NAME)

RN 612528-07-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-08-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-((4-amino-2-bromophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-11-7 HCAPLUS
CN Methanesulfonamide, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612528-12-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-methylphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-09-3 HCAPLUS
CN Acetamide, N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 612528-10-6 HCAPLUS
CN Methanesulfonamide, N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

14 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612528-13-9 HCAPLUS
CN Benzeneacetic acid, α-amino-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}- (9CI) (CA INDEX NAME)

RN 612528-14-0 HCAPLUS
CN Benzeneacetamide, α-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-15-1 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Benzeneacetamide, a-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

RN 612528-16-2 HCAPLUS Benzeneacetamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]- N-propyl- α -[(trifluoroacety1)amino]- (9CI) (CA INDEX NAME)

RN 612528-17-3 HCAPLUS
CN Benzeneacetamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]α-[(methylsulfonyl)amino]-N-propyl- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-20-8 HCAPLUS Benzenepropanamide, α -amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-N-propyl- (9CI) (CA INDEX NAME)

612528-21-9 HCAPLUS
Phenylalanine, N-acetyl-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-18-4 HCAPLUS Benzenepropanamide, α -(acetylamino)-4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-N-propyl- (9CI) (CA INDEX NAME)

612528-19-5 HCAPLUS
Propanedioic acid, (acetylamino)[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-22-0 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -phenyl-, 1,1-dioxide (9C1) (CA INDEX NAME)

612528-23-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2-phenylethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-25-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3,4-dimethoxyphenyl)ethyl]-,
1,1-dioxide
(9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)

RN 612528-26-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(2-chlorophenyl)ethyl]-, 1,1-dioxide
(9CI) (CA INDEX NAME)

RN 612528-27-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(4-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-32-2 HCAPLUS CN 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -(phenylmethyl)-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-33-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[2-(3-aminophenyl)ethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-34-4 HCAPLUS

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-28-6 HCAPLUS
CN Acetamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

RN 612528-29-7 HCAPLUS
CN Butanamide, N-[4-[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)ethyl]phenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(aminomethyl)-1-naphthalenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-35-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(1-ethyl-2-methyl-1H-benzimidazol-5-yl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-36-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-methyl]-1-(3-methylbutyl)-1H-benzimidazol-5-yl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-37-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxy-7-quinolinyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-38-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropoxy);7-quinolinyl|methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612528-19-9 HCAPLUS Glycine, N-[2-(butylamino)-2-oxo-1-phenylethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]- (9CI) (CA INDEX NAME)

612528-40-2 HCAPLUS Glycine, N-[2-(butylamino)-1-(4-ethylphenyl)-2-oxoethyl]-N-[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-42-4 HCAPLUS Glycine, N-[2-(burylamino)-1-(4-methoxyphenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX

PAGE 1-A

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

PAGE 2-A

612528-41-3 HCAPLUS
Glycine, N-[2-(butylamino)-2-oxo-1-(3-phenoxyphenyl)ethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-43-5 HCAPLUS Glycine, N-[1-(2-bromophenyl)-2-(butylamino)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

612528-44-6 HCAPLUS Glycine, N-[2-(butylamino)-1-(2-naphthalenyl)-2-oxoethyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-45-7 HCAPLUS Glycine, N-[2-(butylamino)-1-(4-chlorophenyl)-2-oxoethyl]-N-[4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN NAME) (Continued)

Double bond geometry as shown

RN 612528-48-0 HCAPLUS
CN Glycine,
N-[1-[(burylamino)carbonyl]-3-phenylpropyl]-N-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl)- (9CI) (CA INDEX NAME)

612528-49-1 BCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(methylsulfonyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

612528-46-8 HCAPLUS Glycine, N-[2-(butylamino)-2-oxo-1-[3-(phenylmethoxy)phenyl]ethyl]-N-[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612528-47-9 HCAPLUS
CN Glycine,
N-{(2E)-1-{(butylamino)carbonyl}-3-phenyl-2-propenyl}-N-{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}benzoyl}- (9CI) (CA INDEX

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

612528-50-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(3-chlorophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612528-51-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
(4-butylphenyl]methyl ester (9C1) (CA IMDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612528-53-7 HCAPLUS
CN benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[2-(2-phenylethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

O

H

CH2

CH2

CH2

PAGE 2-A

RN 612528-52-6 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(hydroxymethyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612528-54-8 HCAPLUS CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-, [1,1"-biphenyl)-2-ylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-55-9 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(difluoromethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612528-56-0 HCAPLUS
CN 2-Thiopheneacetic acid,
5-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]benzoyl]oxy]methyl]-α,α-difluoro-(9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612528-59-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[4-[[3-methylbucyl)thio]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me2CH-CH2-CH2-S-

612528-60-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-ethylbutyl ester (9CI) (CA INDEX NAME)

612528-61-7 MCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclobutylmethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612528-57-1 HCAPLUS
Acetic acid, {[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

612528-58-2 HCAPLUS Acetic acid, [[(4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]methyl]thio]-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612528-62-8 HCAPLUS Benzoic acid, 4-[(],1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,cyclopentylmethyl ester (9CI) (CA INDEX NAME)

612528-63-9 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-methylpentyl ester (9CI) (CA INDEX NAME)

612528-64-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2,4,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-65-1 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
cyclohexylmethyl ester (9CI) (CA INDEX NAME)

RN 612528-66-2 HCAPLUS
CM Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-69-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(methylthio)ethyl ester (9CI) (CA INDEX NAME)

RN 612528-70-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-{(carboxymethyl)thio}ethyl ester (9CI) (CA INDEX NAME)

RN 612528-71-9 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
(5-nitro-2-furanyl)methyl ester (9CI) (CA INDEX NAME) .

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-67-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
cyclopentyl ester (9CI) (CA INDEX NAME)

RN 612528-68-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylbutyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612528-72-0 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
2-pyridinylmethyl ester (9C1) (CA INDEX NAME)

RN 612528-73-1 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-chiadiazolidin-2-yl)methyl}-,
[3-(hydroxymethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

- 612528-74-2 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 [3-(methyl]sulfonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

- 612528-76-4 HCAPLUS
 Benzeneacetic acid, 4-{3-{[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}benzoy1}amino]propy1}- {9CI} (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

- 612528-75-3 HCAPLUS
 Benzeneacetic acid, 4-[4-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]benzoy1]amino]buty1]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

- 612528-77-5 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 [5-[(dimethylamino)methyl]-2-furanyl]methyl ester (9CI) (CA INDEX NAME)

- 612528-78-6 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-N-pentyl- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry.

RN 612528-79-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(1H-indol-5-ylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-80-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3,4,5-trimethoxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612528-92-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[4-(phenylmethyl)-1piperazinyl]methyl]phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 612528-85-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(2-naphthalenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612528-86-6 HCAPLUS CN 1,2;5-Thiadiazolidin-3-one, 5-[[4-(4-methyl-1-oxopentyl)phenyl]methyl]-, 1,1-dioxide (901) (CA INDEX NAME)

RN 612528-87-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-(2-fluorophenoxy)phenyl]methyl]-,
1,1-dioxide (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

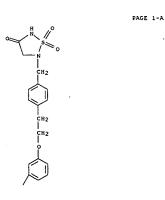
H
O
CH2
CH2
N

RN 612528-83-3 HCAPLUS
CN Benzeneacetic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]- (9CI) (CA INDEX NAME)

RN 612528-84-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-benzoylphenyl)methyl}-, 1,1-dioxide
[9CI] (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-88-8 HCAPLUS
CN Benzoic acid, 3-[2-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl]ethoxyl- (9CI) (CA INDEX NAME)



PAGE 2-A

RN 612528-89-9 HCAPLUS
CN 2(1H)-Quinolinone,
6-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}1-(3-methylbutyl)- (9CI) (CA INDEX NAME)

HO2C

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612528-97-9 HCAPLUS CN Acctamide, 2-amino-N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)methyl]phenyl]methyl] - (9CI) (CA INDEX NAME)

RN 612528-98-0 HCAPLUS

Senzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

(4-carboxyphenyl)methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-00-7 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3nitro- (9CI) (CA INDEX NAME)

RN 612529-01-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-02-9 HCAPLUS CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)nethyl]-, methyl ester (9C1) (CA INDEX MAME) L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

N 612528-99-1 HCAPLUS N 1,2,5-Thiadiazolidin-3-one, 5-[{3-phenoxyphenyl}methyl}-, 1,1-dioxide {9Cl} (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612529-03-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-hydroxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-04-1 HCAPLUS
CN Benzoic acid, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-5nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

HO₂C HO₂C

RN 612529-05-2 HCAPLUS
CN Benzoic acid, 5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

RN 612529-06-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-chloro-3-methoxy-5-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-10-9 HCAPLUS CN 1,2,5-Thladdazolidin-3-one, 5-(3-phenylpropyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-11-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(4-butoxyphenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

H N CH2

RN 612529-12-1 HCAPLUS
CN 1,2,5-thiadiazolidin-3-one, 5-[(2-(trifluoromethyl)phenyl)methyl)-,
1,1-drioxide (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-07-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-nitrophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-08-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methyl-2-nitrophenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

RN 612529-09-6 HCAPLUS

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 612529-13-2 HCAPLUS CN Benzoic acid, 3-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)methyl]- (9C1) (CA INDEX NAME)

RN 612529-14-3 HCAPLUS CN Benzenebutanoic acid, 5-amino-2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)methyl]- (9CI) (CA INDEX NAME)

RN 612529-15-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-methyl-3-nitrophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

1.4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-16-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methyl-3-nitrophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-17-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(5-methyl-2-nitrophenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

RN 612529-22-3 HCAPLUS CN Acetic acid, [[2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2y1)methyl]phenyl]amino]oxo- (9CI) (CA INDEX NAME)

RN 612529-23-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-hydroxyphenyl)methyl]-, 1,1-dioxide
(9C1) (CA INDEX NAME)

RN 612529-24-5 HCAPLUS
CN Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 612529-18-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-aminophenyl)methyl}-, 1,1-dioxide (9CI)
(CA INDEX NAME)

RN 612529-19-8 HCAPLUS
CN 1H-Isoindole-1,3(ZH)-dione,
2-{[4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl|phenyl|methyl|-(9CI) (CA INDEX NAME)

RN 612529-20-1 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione,
2-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 612529-21-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5,5'-[1,4-phenylenebis(methylene)]bis-, 1,1,1'-tetraoxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Conti

RN 612529-26-7 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-fluoro-2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-27-8 HCAPLUS
CN 1,2,5-Thidiazolidin-3-one, 5-[[3-(hydroxymethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-28-9 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-(hydroxymethyl)phenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-29-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(3-amino-4-methylphenyl)methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-30-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-3-methylphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-36-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

612529-37-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-amino-5-hydroxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-31-4 HCAPLUS
1,2,5-Thiadizolidin-3-one, 5-[(3-amino-2-methylphenyl)methyl}-,
1,1-dioxide (9CT) (CA INDEX NAME)

612529-32-5 HCAPLUS
.1,2,5-Thiadiazolidin-3-one, 5-[(2-amino-5-methylphenyl)methyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-33-6 HCAPLUS Acetamide, N-[(14-(i).-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yi]methyl]phenyl]methyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 612529-38-1 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(3,5-dimethylphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

612529-39-2 HCAPLUS
L-Phenylalanine, N-[[3-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenyl}methyl}-, ethyl ester (9CI) (CA INDEX NAME)

612529-40-5 HCAPLUS L-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

612529-41-6 HCAPLUS
Benzoic acid, 2-amino-5-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}-, methy1 ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-42-7 HCAPLUS
CN Benzoic acid,
2-{acctylamino}-4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-43-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-{phenylmethyl}phenyl]methyl}-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-44-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[[2,4-bis(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-45-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,4,6-trifluorophenyl)methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-46-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-bromophenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612529-47-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5,5'-[[1,1'-biphenyl]-2,2'-diylbis(methylene)|bis-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

RN 612529-48-3 HCAPLUS
CN 1,2,5-Thiadia=olidin-3-one, 5-[[4-[(ethylamino)methyl]phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued Benzoic acid, 2-(acetylamino)-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

RN 612529-50-7 HCAPLUS CN Benzoic acid, 2-amino-4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yllmethyl1-, ethyl ester (9CI) (CA INDEX NAME)

RN 612529-51-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(2-phenylethyl)amino]methyl]phenyl]met hyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-52-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[[4-[(diethylamino)methyl]phenyl]methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

612529-53-0 HCAPLUS
Benzoic acid, 2-amino-4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y)|methyl|-, phenylmethyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-57-4 KCAPLUS Benzamide, 4-([1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(3-methylbuyl)- (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-54-1 HCAPLUS
Benzamide, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 612529-56-3 HCAPLUS
CN Benzamide,
4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[2-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-58-5 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -(phenylmethyl)-, 1,1-dioxide, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612529-59-6 HCAPLUS 1,2,5-Thiadiazolidine-2-acetic acid, 4-oxo- α -{phenylmethyl}-, 1,1-dioxide, { α R}- {9CI} (CA INDEX NAME)

612529-60-9 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-61-0 HCAPLUS
CN Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 612529-62-1 HCAPLUS

Senzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-methylpropyl seter (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-65-4 RCAPLUS
CN Benzole acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl)-,
[4-(carboxymethoxy)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

CH₂

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-63-2 HCAPLUS
CN Benzoic acid, 2-amino-4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-64-3 HCAPLUS
CN Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contin

PAGE 2-A

N 612529-67-6 HCAPLUS
N Benzoic acid, 4-[2-[[{4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}methy1]pheny1]methy1]amino]ethy1]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN, 612529-68-7 HCAPLUS
CN Acetic acid, [4-{[1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenoxy}-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

14 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-69-8 HCAPLUS
CN Acetic acid, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]phenoxy]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 612529-70-1 HCAPLUS
RN Benzamide, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl}-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-75-6 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-3-nitro-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612529-76-7 HCAPLUS CN 1.2.5-Thiadiazolidin-3-one, 5-[(4-ethoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME) L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-73-4 HCAPLUS
CN Benzoic acid, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

RN 612529-74-5 HCAPLUS .
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-3-nitro-, ethyl seter (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continu

RN 612529-77-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-{[3-(trifluoromethyl)phenyl]methyl]-,
1,1-dioxide (921) (CA INDEX NAME)

RN 612529-78-9 HCAPLUS
CN Benzeneacetic acid, 4-{{{4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1}benzoy1}oxy|methy1}- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612529-79-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-phenylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

N 612529-82-5 HCAPLUS
N Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl
ester (9C1) (CA INDEX NAME)

RN 612529-83-6 HCAPLUS
CN Benzoic acid, 4+[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-,
2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-80-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(phenylamino)ethyl ester (9CI) (CA INDEX NAME)

RN 612529-81-4 HCAPLUS
CN Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
2-(3-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Co

RN 612529-84-7 HCAPLUS
CN Benzolc acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
3-methoxy-2,2-dimethyl-3-oxopropyl ester (SCI) (CA INDEX NAME)

RN 612529-85-8 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2,2,4-trimethylpentyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-86-9 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
3-(dimethylamino)-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

612529-87-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
[(3aR,4S,5R,6aS)-5-(benzoyloxy)hexahydro-2-oxo-2H-cyclopenta[b]furan-4yl]methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612529-91-6 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(3-chloro-4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 1-A

612529-93-8 HCAPLUS Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiarolidin-2-yl)methyl]-, 6-ethoxy-6-oxohexyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-90-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
(3-methyl-4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

(Continued)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612529-94-9 HCAPLUS
Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-(3-chlorophenyl)ethyl ester (9Cl) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612529-95-0 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiszolidin-2-yl)methyl]-,
2-(3-methyl)henyl)ethyl ester (SCI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

N 612529-96-1 HCAPLUS N Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612529-98-3 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one,
5-[[4-[[(phenylmethyl)amino]methyl]phenyl]meth
yl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Ph-CH2-NH-CH2

RN 612529-99-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)-,
(4-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

14 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-[3-(trifluoromethyl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 612529-97-2 HCAPLUS
CN D-Phenylalanine, N-[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

PAGE 1-A

PAGE 2-A

RN 612530-01-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(methoxycarbonyl)phenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (

(Continued)

PAGE 2-A

RN 612530-02-6 HCAPLUS

Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
2-cyclohexyl-2-methylpropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-04-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

RN 612530-03-7 HCAPLUS
CN Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-phenoxypropyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Con

PAGE 2-A

N 612530-05-9 HCAPLUS
N Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[3-(trifluoromethyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

CF;

RN 612530-06-0 HCAPLUS CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-, 2-(4-carboxyphenyl)ethyl ester (SCI) (CA INDEX NAME) L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 1-A

PAGE 2-A

RN 612530-08-2 HCAPLUS

Benzoic acid, 3-[[[4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

i-BuNH-CH2

RN 612530-10-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(2,2-dimethylpropyl)amino]methyl]pheny l]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Me3C-CH2-NH-CH2

RN 612530-11-7 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
1-naphthalenylmethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 2-A

CO2H

RN 612530-09-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[4-[[(2-methylpropyl)amino]methyl]phenyl]me thyl]-,1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Conti

PAGE 1-A

PAGE 2-A

RN 612530-12-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
(4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 2-A

612530-13-9 HCAPLUS
Benzeneacetic acid, 4-[2-{[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methy1]benzoy1]amino]ethy1]- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

612530-17-3 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
3-[(carboxymethyl)amino]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

612530-18-4 HCAPLUS

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

PAGE 2-A

612530-16-2 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-, (3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl]oxy]methyl]- (9CI) (CA INDEX NAME)

612530-19-5 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
[1,1'-biphenyl}-4-ylmethyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

612530-20-8 HCAPLUS

- ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-,
 [4-(acetylamino)phenyl]methyl ester (9CI) (CA INDEX NAME)
 - PAGE 1-A

PAGE 2-A

PAGE 1-A

- 612530-21-9 HCAPLUS
 Benzoic acid, 4-((1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 [2-(phenylmethyl)phenyl]methyl ester (9C1) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) (2-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

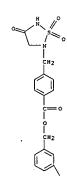
- 612530-25-3 RCAPLUS
 Benzeneacetic acid, 3-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y]]methyl]benzoyl]oxy]methyl]- (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- 612530-22-0 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
 (2-methylphenyl)methyl ester (9CI) (CA INDEX NAME)

- 612530-23-1 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
- ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A



PAGE 2-A

СН2-СО2Н

- 612530-26-4 HCAPLUS
 Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
 (4-methyl-3-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN · (Continued)

PAGE 1-A

612530-27-5 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[4-fluoro-2-(trifluoromethyl)phenyl|methyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

PAGE 1-B

612530-29-7 HCAPLUS
Benzoic acid, 4-{(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl]methyl ester (9CI)
(CA INDEX NAME)

612530-30-0 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)methyl]-, (5-methyl-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

RN 612530-28-6 HCAPLUS
CN Benzoic acid,
4-[{5-{(2,4-dimethoxyphenyl)methyl}-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyll-,
[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)phenyl)methyl ester (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

PAGE 1-A

PAGE 2-A

612530-31-1 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl}-,
2-methylphenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-32-2 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl)-,
3-[(carboxymethyl)methylamino)-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-33-3 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiezolidin-2-yl)methyl]-,
phenyl ester (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-37-7 HCAPLUS
CN 1-Piperazineacetic acid, 4-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]bensoyl]- (9C1) (CA INDEX NAME)

RN 612530-38-8 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 612530-34-4 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-,
[5-[((2-methyl)propyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) (CA
INDEX NAME)

RN 612530-35-5 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
2-naphthalenylmethyl ester (9CI) (CA INDEX NAME)

RN 612530-36-6 HCAPLUS
CN Benzamide, 4-{{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl}-N,N-bis(2-methylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-39-9 HCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[[[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]benzoyl]oxylmethyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 612530-40-2 HCAPLUS
CN Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(aminocarbonyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

RN 612530-41-3 HCAPLUS
CN Piperazine, 1-[4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]benzoyl}-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-42-4 HCAPLUS
Benzoic acid, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-,
[5-(1-oxo-3-phenylpropyl)-2-thienyl]methyl ester (9CI) (CA INDEX NAME)

612530-43-5 HCAPLUS
Benzoic acid, 4-[{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}methyl]-,
[5-[[(phenylmethyl)amino]carbonyl]-2-thienyl]methyl ester (9CI) {CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-48-0 HCAPLUS .
1,2,5-Thiadiazolidin-3-one, 5-[4-{aminomethyl}phenyl]-, 1,1-dioxide {9CI} (CA INDEX NAME)

612530-50-4 HCAPLUS
Benzeneacetic acid, 2-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-(CA INDEX NAME)

612530-51-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-dimethoxyphenyl)-, 1,1-dioxide, potassium salt (9C1) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-44-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-45-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide (9CI) INDEX NAME)

612530-47-9 HCAPLUS
Benzoic acid, 3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA
INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

612530-52-6P 612530-53-7P 612530-54-8P 612530-55-9P 612530-56-0P 612530-57-1P 612530-58-2P 612530-59-3P 612530-60-6P 612530-61-7P 612530-62-8P 612530-63-9P 612530-63-7P 612530-65-1P 612530-66-2P 612530-67-3P 612530-68-4P 612530-69-5P 612530-71-3P 612530-72-0P 612530-73-1P 612530-78-2P 612530-73-9P 612530-73-1P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P 612530-78-6P 612534-93-7P (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (invention compound; preparation of thiazolidinetriones as protein

(invention compound, preparation of thiazolidinetriones as protein tyrosine

phosphatase 1b and T-cell protein tyrosine phosphatase inhibitors to mitigate insulin resistance in the treatment of diabetes or atherosclerosis)

RN 612530-52-6 HCAPIUS

CN Acetamide, 2-{4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1}-3-methylphenoxy}-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

612530-53-7 HCAPLUS 1H-1,4-Benzodiazepine-2,5-dione, 3-[[4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-3-hydroxyphenyl]methyl]-3,4-dihydro-(9CI) (CA

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) NAME)

RN 612530-54-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-(4-iodophenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 612530-55-9 HCAPLUS
CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-56-0 HCAPLUS CN L-Phenylalanine, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 612530-60-6 HCAPLUS
CN L-Phenylalaninamide, N-benzoyl-O-(dicarboxymethyl)-L-tyrosyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-61-7 HCAPLUS
CN Benzenepropanamide, α-{([1,1'-biphenyl]-4-ylsulfonyl)amino]-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 612530-57-1 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-58-2 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-59-3 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-N-[2-{4-(carboxymethyl)phenyl|ethyl]-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continue

RN 612530-62-8 HCAPLUS
CN Benzenepropanamide, a={{[1,1'-bipheny1}-4-ylsulfony1}amino}-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)-, (aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-63-9 HCAPLUS
CN Benzenepropanamide, 4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl}-N-pentyl-a-{{pentyl-a-{{phenylsulfonyl}amino}-, {aS}- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

RN 612530-64-0 HCAPLUS
CN Benzenepropanamide, 4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-y1)-N-(4-phenylbuty1)-a-{(phenylsulfony1)amino}-, (aS)- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 612530-65-1 HCAPLUS
CN Benzenepropanamide,
4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(3,3diphenylpropyl)-a-[(phenylsulfonyl)amino]-, (a\$)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 612530-66-2 HCAPLUS CN L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-Thiadiazolidin-3-one, 5-{(4-aminophenyl)methyl}-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612527-96-5 CMF C9 H11 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612530-72-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{{1-ethyl-2-methyl-1H-benzimidazol-5-yl}methyl}-, 1,1-dioxide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 612528-35-5 CMF C13 H16 N4 O3 S

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-67-3 HCAPLUS Benzenepropanamide, 3-bromo-4-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-(4-phenylbutyl)- α -[(phenylsulfonyl)amino}-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-68-4 HCAPLUS L-Phenylalaninamide, etyl-L-Phenylalanyl-3-bromo-4-{1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

612530-69-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

612530-71-9 HCAPLUS

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CM 2

612530-73-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[{4-{(2)-(3-oxo-2(3H)-benzofuranylidene)methyl}phenyl}methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

612530-74-2 HCAPLUS Ethanedione, [4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]phenyl]phenyl- (9CI) (CA INDEX NAME)

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

612530-75-3 HCAPLUS
9,10-Anthracenedione, 2-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl)- (9CI) (CA INDEX NAME)

612530-77-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-phenyl-, 1,1-dioxide, sodium_salt (9CI) INDEX NAME)

612530-78-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-(2,4-diaminophenyl)-, 1,1-dioxide, trifluoroacetate (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN (COntinued)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 1

CRN 612530-45-7 CMF CB H10 N4 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

612534-93-7 HCAPLUS L-Phenylalaninamide, N-acetyl-L-phenylalanyl-3-(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)-N-pentyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 31 Jul 2002
ACCESSION NUMBER: 2002:55367 HCAPLUS
ITILE: Efficient Solid-Phase Synthesis of Sulfahydantoins
AUTHOR(S): Efficient Solid-Phase Synthesis of Sulfahydantoins
Tremblay, Nelanie: Voyer, Normand: Boujabi, Sihem,
Dewynter, Georges F.
Centre de Recherche sur la Fonction, la Structure et
l'Ingenierie des Proteines, Departement de Chimie,
Faculte des Sciences et de Genie, Universite Laval,
Quebec, OC, GLK 7P4, Can.
Journal of Combinatorial Chemistry (2002), 4(5),
429-435
CODEN: JCCHFF; ISSN: 1520-4766
American Chemical Society
Journal
LANGUAGE: July JCCHFF; ISSN: 1520-4766
American Chemical Society
Journal
English
CTHER SOURCE(S): CASREACT 137:232603

AB A novel solid-phase strategy allows the efficient preparation of traceless sulfahydantoins. A total of 28 derivs, with crude purity generally higher than 85%, were prepared by parallel synthesis. Through reductive alkylations, Mitsunobu reactions, and sulfamoylation reactions on oxime resin, the synthetic strategy affords sulfahydantoin deriva. selectively substituted at N2, e.g., I, N5, e.g., II, and N2, N5, e.g., III, positions, slthough yields of disubstituted compds. are lower. The mild reaction conditions involved, lead to sulfahydantoins without racemization.

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
459831-33-5P 459831-34-6P 459831-35-7P
RL: SPN (Synthetic preparation) PREP (Preparation)
(stereoselective preparation of N2,N5-disubstituted sulfahydantoins

reductive alkylation of resin-bound phenylalanine with substituted benzaldehydes and subsequent sulfamoylation, Mitsunobu reaction, resin-cleavage, and cyclization)

RN 459831-33-5 MCAPUUS

CN 1,2,5-Thiadiazolidin-3-one,
5-{(4-methylbenyl|methyl)-4-{phenylmethyl}-2{2-propenyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-34-6 HCAPLUS
1,2,5-Thiadiazolidin-3-ońe, 2-butyl-5-[(4-methylphenyl)methyl]-4(phenylmethyl)-, 1,1-dioxide, (45)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

RN 459831-35-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methylphenyl)methyl]-4-[phenylmethyl]-2(3-phenylpropyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 283587-14-4P 459831-30-2P 459831-31-3P 459831-32-4P (Continued) 459831-32-4P RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective preparation of N5-substituted sulfahydantoins via nuctive
 alkylation of resin-bound phenylalanine with substituted benzaldehydes
 and subsequent sulfamoylation, resin-cleavage, and cyclization)
283587-14-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methoxyphenyl)methyl]-4-(phenylmethyl)-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

459831-30-2 HCAPLUS TOFORTON TO THE TOTAL TO THE TOTAL TO THE TOTAL THE

Absolute stereochemistry.

459831-31-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-nitrophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

459831-32-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-methylphenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 Oct 2001
ACCESSION NUMBER: 2001:735235 HCAPLUS
DOCUMENT NUMBER: 136:85785
TITLE: 4 A one-step protocol for the N-chloromethylation of heterocyclic imides
AUTHOR(S): He, Shu; Yu, Hongyi; Fu, Qinghong; Kuang, Rongze;

AUTHOR(S): Epp,

CORPORATE SOURCE:

Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA

SOURCE:

SOURCE:

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

DOLINER SOURCE(S):

AB A convenient single step methodol. for the N-chloromethylation of heterocyclic imides using a mixture of formaldehyde sodium bisulfite adduct

and thionyl chloride is described. For example, the chloromethylation of 5-Butyl-3-propyl-1,2,5-thiadiazolidin-3-one 1,1-dioxide gave. 387859-83-8 387859-86-1 RACT (Reactant) reagent) (preparation of 2-(chloromethyl)-1,2,5-thiadiazolidin-3-one by chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 387859-83-8 HCAPLUS 1,2,5-thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 387859-86-1 HCAPLUS CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

300553-85-9P 387859-88-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-{chloromethyl}-1,2,5-thiadiazolidin-3-one by

ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) chloromethylation of 1,2,5-thiadiazolidin-3-one using thionyl chloride and formaldehyde sodium bisulfite adduct) 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

387859-88-3 HCAPLUS 1,2,5-Thiadiazolidine-3-acetic acid, 5-(chloromethyl)-4-oxo-2-(phenylmethyl)-, phenylmethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester (9C1) (CA INDEX

220869-14-7 HCAPLUS

220869-16-9 HCAPLUS

[2-[[[4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 13 Jun 2001 ACCESSION NUMBER: 2001:426029 HCAPLUS DOCUMENT NUMBER: 135:282665

TITLE: Inhibition of serine proteases by functionalized sulfonamides coupled to the

1,2,5-thiadiazolidin-3-one

ne
1,1 dioxide scaffold
Groutas, W. C.; He, S.; Kuang, R.; Ruan, S.; Tu, J.;
Chan, H.-K.
Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry (2001), 9(6),
1543-1548 AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE: AB A challen

ABA A challenge associated with drug design is the development of selective Inhibitors of processes (serime or cysteine) that exhibit the same primary substrate specificity, i.e., show a preference for the same P1 residue. While these processes have similar active sites, nevertheless there are subtle differences in their 3 and 8' subsites which can be exploited. We describe herein for the first time the use of functionalized sulfonamides as a design and diversity element which, when coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold yields potent, time-dependent inhibitors of the serime proteases human leukocyte elastase

(HLE), proteinase 3 (PR 3) and cathepsin G (Cat G). Our preliminary findings suggest that (a) appending to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold recognition and diversity elements that interact with both the S and S' subsites of a target protease may result in optimal enzyme selectivity and potency and, (b) functionalized sulfonamides constitute a powerful design and diversity element with low intrinsic chemical reactivity and potentially wide applicability. Potent inhibitors of human leukocyte elastase, proteinase 3 and cathepsin G that interact with the S and S' subsites are realized by using functional sulfonamides coupled to the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold.

12 20869-05-69 20869-07-69 220869-07-69 220869-01-47P 220869-05-69 220869-01-69 220869-01-69 20869-01-69 20869-01-69 20869-01-69 BESIG-03-9P RL: BAC (Biological activity or effector, except adverse); BSU (Therspeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (Uses)

ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 1,2,5-thiadiazolidin-2-yllmethyl(methylsulfonyl)amino]-2-oxoethyl)-,phenylmethyl ester (9C1) (CA INDEX NAME)

RN 365216-39-3 HCAPLUS
CN Benzamide,
N-[{4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

365216-41-7 HCAPLUS

Glycine,
[[[[4-(2-methylpropy1)-1,1-dioxido-3-oxo-5-[phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carbonyl]-, ethyl ester
(9CI) (CA INDEX NAME)

365216-42-8 HCAPLUS

L4 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Carbamic acid, {[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}(phenylsulfonyl)-, butyl ester (9CI) (CA
INDEX
NAME)

RN 365216-43-9 HCAPLUS
CN L-Phenylalanine, N-[[[[(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-

(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)amino]carb onyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

35

REFERENCE COUNT: THIS

THERE ARE 35 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 283587-15-5 HCAPLUS CN 1,2,5-Thidiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (45)- (901) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-16-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-(13-methylphenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 283587-19-9 HCAPLUS

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN • ED Entered STN: 24 Apr 2001
ACCESSION NUMBER: 135:76831
TITLE: AUTHOR(S): Albericio, Fernando; Bryman, Lois M.; Garcia, Javier; Michelotti, Enrique L.; Nicolas, Enresto; Tice, Colin M.

CORPORATE SOURCE: Department of Organic Chemistry, University of Barcelona, Barcelona, 08028, Spain Journal of Combinatorial Chemistry (2001), 3(3), 290-300
CODEN: JCCNFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
JOURNAL AMERICAN CHEMICAL SOURCE(S): CASREACT 135:76831
AB A five-step solid-phase synthesis of sulfahydantoins from α-amino acids and aldehydes was developed. The synthetic method allows the use of hindered amino acids, including Val, Phe, and Alb, and use of aromatic aldehydes substituted with electron-withdrawing and -donating groups. Some limitations were encountered with amino acids with reactive side chains. A small but diverse library of compds. was produced for biol. testing.

I7 283587-18-8P 283587-19-9P 283587-21-6P 283587-18-8P 346697-39-0P 346697-43-P 346697-51-P 3

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued I, 2,5-Thiadiazolidin-3-one, 5-{(2,3-dihydro-1,4-benzodioxin-6-y1)methyl}-4-(1-methylethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiszolidin-3-one, 5-{(2-chlorophenyl)methyl)-4-{1-methylethyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 283587-22-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 283587-24-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-(2-(methylthio)ethyl]-, 1,1-dioxide, (4S]- (9CI) (CA INDEX NAME)

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-35-6 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-((3-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

346697-36-7 HCAPLUS
Acetamide, N-(4-[(35)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-37-8 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(1-methyl)tchyl)-5-(6-nitro-1,3-benzodioxol5-yl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-42-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4-[[4[phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI)- (CA INDEX NAME)

Absolute stereochemistry.

Seebs/43-5 NCAPUS
Acetamide, N-(4-[[(35)-1,1-dioxido-4-oxo-3-[[4(phenylmethoxy)phenyl]methyl]-1,2,5-thiadiazolidin-2-yl]methyl]phenyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346697-38-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

RN 346697-39-0 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[[2-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-40-3 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl}-4-(1-methylethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

346697-41-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2-chlorophenyl)methyl]-4-[[4(phenylmethoxy)phenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

346697-45-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl)-4-[(4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} Ph & C & \\ \hline \\ S & N \\ \hline \end{array}$$

RN 346697-46-9 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,4-dimethoxy,3-methylphenyl]methyl]-4-[(4(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-47-0 RCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl)-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN . (Continued)

346697-48-1 RCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

RN 346697-49-2 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl]-4-[2-(methylthio)ethyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

RN 346697-50-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[[2-chloro-5-(trifluoromethyl]phenyl]methyl]4-[2-(methylthio)ethyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
346697-55-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(6-nitro-1,3-benzodioxol-5-yl]methyl]-4[([phenylmethyl]thio]methyl)-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-56-1 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 5-[(4-chloro-3-nitrophenyl)methyl]-4[((phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-57-2 HCAPLUS
1,2,5-Thiadiarollidine-3-acetic acid, 2-[(3-chlorophenyl)methyl)-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-58-3 HCAPLUS
1,2,5-Thiadiszolidine-3-acetic acid, 2-[[4-(acetylamino)phenyl]methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (38)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-51-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one,'5-[(2-chlorophenyl)methyl]-4[(jberylnethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

346697-53-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(3-chlorophenyl)methyl]-4[[(phenylmethyl)thio)methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

346697-54-9 HCAPLUS
Acetamide, N-{4-[{(3R}-1,1-dioxido-4-oxo-3-[{(phenylmethyl)thio]methyl]-1,2,5-thiadiazolidin-2-yl]methyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 346697-59-4 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid,
2-[(4-chloro-3-nitrophenyl)methyl]-4oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-60-7 HCAPLUS
1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2,4-dimethoxy-3-methylphenyl)methyl]-4-oxo-, phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

RN 346697-62-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chlorophenyl)methyl)-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-63-0 HCAPLUS
(1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-64-1 HCAPLUS
CN 1,2,5-Thiadiarolidin-3-one, 4-(1-methylethyl)-5-[(3-(trifluoromethyl)phenyl]methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-65-2 HCAPLUS
CN Benzoic acid, 4-[[(3S)-3-(1-methylethyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-73-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[{2-chioro-5-(trifluoromethyl)phenyl]methyl}4-[{4-(phenylmethoxy)phenyl]methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-74-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[[1-(phenylmethyl)-1H-imidazol-4-yl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-75-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-[[1-(phenylmethyl)-1H-imidazol-4-yl]methyl]- L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-69-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[(3-methylphenyl)methyl]-4-[(4(phenylmethoxylphenyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-71-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[[4-(phenylmethoxy)phenyl]methyl]-5-[[4-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-72-1 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[(4-(phenylmethoxy)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
5-[(4-(trifluoromethyl)phenyl)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-76-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[[1-(phenylmethyl)-1H-imidazol-4-yl)methyl]-, 1,1-dioxide, (4S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry

RN 346697-77-6 HCAPLUS

1,2,5-Thiadiazolidine-3-acetic acid, 2-[(3-methylphenyl)methyl]-4-oxo-, methyl ester, 1,1-dioxide, (33)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-79-8 HCAPLUS

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-[[4(trifluoromethyl)phenyl]methyl]-, methyl ester, 1,1-dioxide, (3S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 346697-80-1 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-{(2,3-dihydro-1,4-benzodioxin-6-yl)methyl}-4-oxo-, methyl ester, 1,1-dioxide, '(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-81-2 HCAPLUS
CN Acetamide, N-[4-[([35]-3-[2-(methylthio)ethyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]phenyl]- [9C1) (CA INDEX NAME)

Absolute stereochemistry

RN 346697-82-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-[2-(methylthio)ethyl]-5-{(6-nitro-1,3-benzodioxol-5-yl)methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 346697-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(2-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-87-8 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(4-chlorophenyl)methyl]-4-oxo-,
phenylmethyl ester, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-88-9 HCAPLUS
CN 1,2,5-Thiadiazolidine-3-acetic acid, 2-[(6-nitro-1,3-benzodioxol-5-y1)methyl-4-oxo-, phenylmethyl ester, 1,1-dioxide, (3S)- (9CI) (CFINDEX

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346697-03-4 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-[(4-chlorophenyl)methyl)-4-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 346697-84-5 HCAPLUS
N 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dimethoxy-3-methylphenyl)methyl]-4[[(phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-85-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(2-chloro-5-(trifluoromethyl)phenyl]methyl]4-[([phenylmethyl)thio]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

RN 346697-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-{{phenylmethoxy}methyl}-5-{{2-(trifluoromethyl)phenyl}methyl}-, 1,1-dioxide, (4S}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346697-91-4 HCAPLUS
CN 1.2.5-Thiadiacolidin-3-one, 4-{(phenylmethoxy)methyl}-5-[[3-(trifluoromethyl)phenyl)methyl]-, 1.1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-92-5 HCAPLUS
Benzoic acid, 4-{{(3S)-1,1-dioxido-4-oxo-3-{(phenylmethoxy)methyl}-1,2,5-thiadiazolidin-2-yl]methyl}-, methyl ester (9CI) (CA INDEX NAME)

346697-93-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dichlorophenyl)methyl}-4[(phenylmethoxy)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

346697-97-0 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[2-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 346698-03-1 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-phenyl-5-[(2-(trifluoromethyl)phenyl)methyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 346698-04-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-phenyl-5-[[3-(trifluoromethyl)phenyl]methyl], 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-05-3 HCAPLUS
Benzoic acid, 4-[((35)-1,1-dioxido-4-oxo-3-phenyl-1,2,5-thiadiazolidin-2-yllmethyll-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

346697-98-1 HAPLUS
1,2,5-Thiadiazolidin-3-one, 4-[(4-nitrophenyl)methyl]-5-[[3-(trifluoromethyl)phenyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346697-99-2 HCAPLUS
Benzoic acid, 4-[(SS)-3-[(4-nitrophenyl)methyl]-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

346698-00-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-[(4-nitrophenyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 346698-06-4 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2,3-dichlorophenyl)methyl]-4-phenyl-1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

346698-14-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4-[(15)-1-methylpropyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 47 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Dec 2000
ACCESSION NUMBER: 2000:898004 HCAPLUS
DOCUMENT NUMBER: 134:307088

TITLE: 1,2,5-Thiadiazolidin-3-one 1,1 Dioxide: A Powerful Scaffold for Probing the 5' Subsites of (Chymo)trypsin-Like Serine Proteases

AUTHOR(S): Groutas, William C.; Epp, Jeffrey B.; Kuang, Rongze; Ruan, Sumei; Chong, Lee S.; Venkataraman, Radhika;

Tu,

Juan; He, Shu; Yu, Hongyi; Fu, Qinghong; Li, Yue He;
Truong, Tien M.; Vu, Nga T.

CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA

SOURCE: Archives of Biochemistry and Biophysics (2001),
385(1), 162-169
CODEN: ABBIA4; ISSN: 0003-9861

PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: Argish
B The 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (I) embodies a motif
that allows it to dock to the active site of (chymo)trypsin-like

nases in a predictable and substrate-like fashion. Consequently, inhibitors derived from this heterocyclic scaffold interact with both the S and S subsites of an enzyme. Exploitation of binding interactions with both

S and S' subsites of a target enzyme may lead to compds. With greatly enhanced enzyme selectivity and inhibitory potency. This preliminary report describes the use of a series of compds. having the heterocyclic scaffold linked to various amino acids to probe the S' subsites of human leukocyte elastase (HLE), proteinase 3 (PR 3), and cathepsin G (Cat G). For comparative purposes, a series of compds. derived from a related scaffold, isothiazolidin-3-one 1,1 dioxide (III), was also generated. Several of the compds. were found to be highly potent and selective time-dependent inhibitors of HLE, PR 3, and Cat G. (c) 2001 Academic

78-334975-68-7P 334975-69-8P 334975-75-6P 334975-81-4P 334975-83-6P 334975-85-8P 334975-85-8P

RL: BAC (Biological activity or effector, except adverse); BSU

logical study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (BiOLogical study); PREP (Preparation) (1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold for probing S' subsites of human leukocyte elastase, proteinase 3 and cathepsin G) 334975-68-7 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(4S)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

со2н

334975-81-4 HCAPLUS L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, {(4S)-1,1-dioxido-3-ox-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-83-6 HCAPLUS
L-Phenylalanine, ((45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5
thiadiazolidin-2-yl]methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

334975-69-8 HCAPLUS
D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

334975-75-6 HCAPLUS

3349/3-73-6
L-Phenylalanine, [(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yllmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 334975-74-5 CMF C23 H29 N3 O5 S

Absolute stereochemistry

ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) D-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, [(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

334975-88-1 HCAPLUS
D-Phenylalanine, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: THERE ARE 24 CITED REFERENCES AVAILABLE FOR

L4 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 220869-27-2 HCAPLUS
CN 1.2.5-Thiadiazolidin-3-one,
2-[[(4.5-diphenyl-2-oxazoly1)thio]methyl}-4-(2methylpropyl)-5-(phenylmethyl)-, 1.1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide (9CI) (CA INDEX

L4 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 19 Jul 2000 ACCESSION NUMBER: 2000:488727 HCAPLUS

DOCUMENT NUMBER:

133:277919
Potent inhibition of serine proteases by heterocyclic sulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1 TITLE:

sulfide derivatives of 1,2,5-thiadiazolidin-3-one 1,1 dioxide
AUTHOR(S): He, S.; Kuang, R.; Venkataraman, R.; Tu, J.; Truong, T. M.; Chan, H. K.; Groutas, W. C.

CORPORATE SOURCE: Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
SOURCE: Bicorganic & Medicinal Chemistry (2000), 8(7), 1713-1717

CODEN: BMECEP, ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASPRACT 133:277919
AB The existence of subtle differences in the Sn' subsites of closely-related
(chymo)trypsin-like serine proteases, and the fact that the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold docks to the active site of (chymo)trypsin-like enzymes in a substrate-like fashion, suggested that

that the introduction of recognition elements that can potentially interact with the Sn' subsites of these proteases might provide an effective means for optimizing enzyme potency and selectivity. Accordingly, a series of heterocyclic sulfide derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold (1) was synthesized and the inhibitory activity and selectivity of these compds. toward human leukocyte elastase (HLE), proteinase 3 (PR 3) and cathepsin G (Cat G) were then determined Compds. with Pleisobutyl were found to be potent, time-dependent inhibitors of HLE and,

Pleisobutyl were found to be potent, time-dependent inhibitors of HLE and,
to a lesser extent PR 3, while those with Pl-benzyl inactivated Cat G
rapidly and irreversibly. This study has demonstrated that
1,2,5-thiadiazolidin-3-one 1,1 dioxide-based heterocyclic sulfides are
effective inhibitors of (chymoltypsin-like serine proteases.

IT 220869-26-1P 220869-37-2P 220869-35-2P
220869-30-7P 220869-33-9-8P 220869-35-2P
220869-38-5P 220869-39-6P 220869-40-9P
RL: BAC (Biological activity or effector, except adverse): BSU
(Biological
study): PREP (Preparation)
(potent inhibition of serine proteases by heterocyclic sulfide derivs.
of thiadiazolidinone dioxide)
RN 220869-26-1 RCRPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-((2-benzoxazolylthio)methyl)-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) 220869-30-7 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-[phenylmethyl]-, 1,1-dioxide (9C1) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-35-2 HCAPLUS 1,2,5-Thiadiarolidin-3-one, 4-(2-methylpropyl)-2-[[(5-phenyl-2-benzoxazolyl)thio]methyl]-5-[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[phenylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

(Continued) ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

220869-39-6 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 4,5-bis(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxediazol-2-yl)thio)methyl)-, 1,1-dioxide (SCI) (CA INDEX NAME)

220869-40-9 HCAPLUS
1,2,3-Thiadiacolidin-3-one, 2-[[(6-amino-2-benzoxazolyl)thio|methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

IT

300553-85-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of thiadiazolidinone dioxide derivative; potent inhibition

serine proteases by heterocyclic sulfide derivs. of thiadiazolidinone dioxide)

L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 15 Jun 2000 ACCESSION NUMBER: 2000:395930 HCAPLUS

133:159638

Utilization of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold in the design of potent inhibitors TITLE:

AUTHOR (S):

Serine proteases: SAR studies using carboxylates Kuang, R.; Epp, J. B.; Ruan, S.; Chong, L. S.; Venkataraman, R.; Tu, J.; He, S.; Truong, T. M.; Groutas, W. C.
Department of Chemistry, Wichita State University, Wichita, KS, 61260, USA
Bioorganic & Medicinal Chemistry (2000), 8(5), 1005-1016
CODEN: BMECEP; ISSN: 0968-0896
Elsevier Science Ltd.
Journal CORPORATE SOURCE:

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE :

MENT TYPE: Journal UAGE: English A series of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds has been synthesized and the inhibitory profile of these compds. toward human leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3) was then determined Most of the compds. were found to be potent,

then determined Most of the compds. were found to be potent, -dependent inhibitors of elastase, with some of the compds. exhibiting kinact/KI values as high as 4,928,300 M-1 s-1. The inhibitory potency of carboxylate derivs. based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide platform was found to be influenced by both the pKs and the inherent structure of the leaving group. Proper selection of the primary specificity group was found to lead to selective inhibition of HLE over Cat G, however, those compds. that inhibited HLE also inhibited PR 3, albeit less efficiently. The predictable mode of binding of these dds.

ds.
suggests that, among closely-related serine proteases, highly selective inhibitors of a particular serine protease can be fashioned by exploiting subtle differences in their S' subsites.
247179-63-1P 287921-30-6P 287921-33-9P 287921-73-79 287921-73-8P 287921-73-8P 287921-82-0P 287921-45-3P 287921-46-4P 287921-65-7P 287921-91-9P

RL: BAC (Biological activity or effector, except adverse); BSU

logical study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis of thiadiazolidinone dioxides and isothiazolidinone

as serine protease inhibitors)
247179-63-1 HCAPLUS

1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-4,5-bis(phenylmethyl)-,
1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 300553-85-9 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME) (Continued)

THERE ARE 27 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-30-6 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-,
[4-ethyl-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-33-9 HCAPLUS
Benzeneacetic acid, 4-[[(35)-5-[(2,2-dimethyl-1-oxopropoxy)methyl]-1,1-dioxido-4-oxo-3-propyl-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA

INDEX

NAME)

Absolute stereochemistry.

RN 287921-37-3 HCAPLUS
Propanoic acid, 2,2-dimethyl-,
[(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

, L4 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

287921-38-4 HCAPLUS
Benzeneacetic acid, 4-[[(3S)-5-[{2,2-dimethyl-1-oxopropoxy)methyl}-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

287921-39-5 HCAPLUS Zerzzi-39-3 KCAPUUS 1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-42-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{{benzoyloxy}methyl}-4-{2-methylpropyl}-5-{phenylmethyl}-, 1,1-dioxide, (4S)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Benzenepropanoic acid, [(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

287921-54-4 HCAPLUS
Benzeneacetic acid, [(45)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

287921-65-7 HCAPLUS
Benzoic acid, 2,6-dichloro-,
-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)1,2,5-thiadiazolidin-2-yl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-91-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{(acetyloxy)methyl}-4,5-bis(phenylmethyl)-,1,1-dioxide(9CI) (CA INDEX NAME)

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 287921-45-3 HCAPLUS
CN Benzoic acid, 2,6-dichloro-,
[(48)-4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-46-4 HCAPLUS
Benzeneacetic acid, 4-[[(3S)-5-[[{2,6-dichlorobenzoyl)oxy]methyl]-3-(2-methylpropyl)-1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

287921-52-2 HCAPLUS

ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

212331-98-1P 212331-99-2P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (synthesis of thiadiazolidinone dioxides and isothiazolidinone IT

dioxides

ides
as serine protease inhibitors)
212331-98-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2(phenylthio)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-99-2 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 44 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: THIS

FORMAT

L4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 May 2000
ACCESSION NUMBER: 2000:324184 HCAPLUS
COUCHENT NUMBER: 133:105000
TITLE: Solid-phase synthesis of sulfahydantoins
Albericio, Fernando; Garcia, Javier; Michelotti,
Enrique L.: Nicolas, Ernesto: Tice, Colin M.

CORPORATE SOURCE: Department of Organic Chemistry, University of
Barcelona, Barcelona, 08028, Spain
Tetrahedron Letters (2000), 41(17), 3161-3163
CODEN: TELEATY, ISSN: 0040-4039
PUBLISHER: Disavier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: CASRACT 133:105000
OTHER SOURCE(S): CASRACT 133:105000
AB A 5-step solid-phase synthesis of 2-unsubstituted 1,2,5-thiadiazolidin-3one 1,1-dioxides, sulfahydantoins, from Nu-Faoc amino acids and
aromatic aldehydes is described. The key step is the base-mediated
cyclitive

aromatic aldehydes is described. The key step is the Dass-medicipalities

cleavage of a resin bound Nu-minrosulfonyl Nu-benzyl amino
acid to afford the desired product. This synthesis allows the
preparation of a
diverse library of compds. based on this heterocycle.

IT 283587-14-4P 283587-15-5P 283587-16-6P
283587-18-8P 283587-19-9P 283587-21-3P
283587-12-4P 283587-14-9P 283587-21-3P

[solid-phase synthesis of sulfahydantoin library]

RN 283587-14-4 MCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-[(4-methoxyphenyl)methyl)-4-(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCAPLUS 1,2,5-Thiadiazolidin-3-one, 5-[(2,4-dichlorophenyl)methyl]-4-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 283587-21-3 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2-chlorophenyl)methyl}-4-(1-methylethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-22-4 HCAPLUS 1,2,5-Thiadiacolidin-3-one, 5-[(4-methoxyphenyl)methyl]-4,4-dimethyl-,1,1-dioxide (9CI) (CA INDEX NAME)

283587-24-6 HCAPLUS 1,2,5-Thiadizalidin-3-one, 5-((2-chlorophenyl)methyl)-4-(2-(methylthio)ethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1.4 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

283587-16-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, -methylethyl)-5-[(3-methylphenyi)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

283587-18-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-{{4-(trifluoromethyl)phenyl}methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN . 283587-19-9 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 5-{(2,3-dihydro-1,4-benzodioxin-6-y1)methy1}-4-{1-methylethy1}-, 1,1-dioxide, {45}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 27 Aug 1999
ACCESSION NUMBER: 1999:536684 HCAPLUS
DOCUMENT NUMBER: 131:296963
TITLE: 131:296963
AUTHOR(S): Human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold Groutes, William C.; Schechter, Norman M.; He, Shu; Yu, Hongyi; Huang, Peng; Tu, Juan
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1999), 9(15), 2199-2204
CODEN: BMCLEB: ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANCUAGE: English
AB A series of compds. that utilize the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold was synthesized and shown to be highly effective inhibitors of recombinant human skin chymase..

IT 170918-99-7 247178-61-2 247179-63-1
247179-64-2 247179-64-6 247179-66-4
247179-70-0 247179-71-75-5 247179-76-6
RL: BBAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); PRP (Properties); BIOL (Biological study) (human chymase inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1 dioxide scaffold)
RN 170918-99-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[((4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN CN Acetic acid, hydroxy-, [(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry.

RN 247179-66-4 HCAPLUS CN Propanoic acid, 2-hydroxy-, [(45)-1,1-dioxido-3-oxo-4,5-bis[phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-67-5 HCAPLUS
Benzenescetic acid, a-hydroxy-, ((48)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thladiazolidin-2-yl]methyl ester (9CI) (CA INDEX

Absolute stereochemistry.

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-63-1 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-{{acetyloxy}methyl}-4,5-bis(phenylmethyl)-,
1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-64-2 HCAPLUS
Propanedioic acid, mono[[(4S)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-65-3 HCAPLUS

ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

247179-68-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(methylsulfonyl)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-69-7 HCAPLUS
Acetic acid, [[[(4\$)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

247179-70-0 HCAPLUS
Propanoic acid, 3-[[[{45}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

247179-71-1 HCAPLUS
Benzoic acid, 2-{{{(4S}-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl}sulfonyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-72-2 HCAPLUS
Benzoic acid, 3-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yllmethyl)aulfonyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: THIS

THERE ARE 25 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247179-74-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-75-5 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 2-[((6-amino-2-benzoxazolyl)thio]methyl]-4,5-bis(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247179-76-6 HCAPIUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl}-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 25 Aug 1999
ACCESSION NUMBER: 1999:529836 HCAPLUS
DOCUMENT NUMBER: 131:296959
TITLE: A General Inhibitor Scaffold for Serine Proteases
with

TITLE:

A General Inhibitor Scaffold for Serine Proteases with

a (Chýmo)trypsin-Like Fold: Solution-Phase Construction and Evaluation of the First Series of Libraries of Mechanism-Based Inhibitors

AUTHOR(S):

Kuang, Rongze: Epp. Jeffrey B.: Ruan, Sumei; Yu, Hongyi: Huang, Peng; He, Shu: Tu, Juan: Schechter, Norman M.: Turbov, Jane: Froelich, Christopher J.: Groutas, William C.

CORPORATE SOURCE:

Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA

SOURCE:

Journal of the American Chemical Society (1999), 121(35), 8128-8129

CODEN: JACSAT; ISSN: 0002-7863

American Chemical Society

DOCUMENT TYPE:

DOCUMENT TYPE:

DATE American Chemical Society

DOCUMENT TYPE:

LANGUAGE:

AB The authors demonstrate that the 1,2,5-thiadiazolidin-3-one 1,1 dioxida platform embodies a general motif that renders the platform capable of binding to the active size of many serine proceases with a (chymo)trypsin-like fold in a predictable fashion and is amenable to the facile construction of libraries for lead identification and optimization.

facile construction of libraries for lead identification and optimization.

IT 170918-99-7P 170919-03-6P 189124-02-5P 247178-39-8P 247178-40-12P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (inhibitor; general inhibitor scaffold for serine proteases with a (chymo)trypsin-like fold with solution-phase construction and evaluation

evaluation

of first series of libraries of mechanism-based inhibitors)

RN 170918-99-7 HCAPLUS

CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2{(phenylaulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN Absolute stereochemistry. (Continued)

RN 189124-02-5 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
5-(phenylmethyl)-2-((phenylsulfonyl)methyl]-4propyl-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-39-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(4-aminobutyl)-5-(phenylmethyl)-2[(phenylmultonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 16 Mar 1999
ACCESSION NUMBER: 1999:172588 HCAPLUS
130:209985
TITLE: Preparation of 1,2,5-thiadiazolidin-3-one 1,1-dioxide derivatives as serine protease inhibitors
INVENTOR(S): Groutas, William C.; Kuang, Rongze
PATEMT ASSIGNEE(S): Wichita State University, USA
SOURCE: COEN: PIXXD2
DOCUMENT TYPE: Patemt
LANGUAGE: Patemt
LANGUAGE: Bnglish
FAMILY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	ICATION NO.	DATE
WO 9909977 Al 19990304 WO 1		
WO 9909977 A1 19990304 WO 1		
	998-US17406	19980821
W: AU, BR, CA, IS, JP, MX, NZ		
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR,	GB, GR, IE, IT,	LU, MC, NL,
PT, SE		
US 6420401 B1 20020716 US 1	997-916693	19970822
AU 9890298 A 19990316 AU 1	998-90298	19980821
EP 1011668 A1 20000628 EP 1	998-942192	19980821
R: DE, GB		
RIORITY APPLN. INFO.: US 1	997-916693	A 19970822
NO 1	998-US17406	w 19980821

OTHER SOURCE(S):

MARPAT 130:209985

L4 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

247178-40-1 HCAPLUS

1,2,5-Thiadiazolidine-3-acetic acid, 4-oxo-2-(phenylmethyl)-5-[(phenylsulfonyl)methyl)-, 1,1-dioxide, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

247178-41-2 HCAPLUS
Benzoic acid, 4-[[[(45)-1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) = G, H; m = 1-2; each R7 = amino acid side chain; each R8, R9 = alkyl, aryl, aralkyl, alkaryl, heterocyclyl; each R10-R15 = H, any group R8;

R16, R17 = heterocyclylalkyl; R16 = any group R8, NHR19; R19 = alkyl, aryl, aralkyl; with provisos], oligomers and combinatorial libraries contg. them, and methods of using them, are disclosed. Thus, title

contg. them, and methods of using them, are disclosed. Thus, title d.

II showed apparent second-order rate consts. Kinact/KI (Mrls-1) of 119,360, 27,400, and 60 for inhibition of human leukocyte elastase, proteinase 3, and catheppin G, resp., by in vitro assays. 220868-4-6DP, combinatorial library derivs. 220868-75-7DP, combinatorial library derivs. 220868-81-5DP, combinatorial library derivs. 220868-81-5DP, combinatorial library derivs. 220868-86-6DP, combinatorial library derivs. 220868-81-5DP, combinatorial library derivs. 220868-93-DPP, combinatorial library derivs. 220868-93-9DP, combinatorial library derivs. 220868-93-6DP, combinatorial library derivs. 220868-93-5DP, combinatorial library derivs. 220868-93-5DP, combinatorial library derivs. 220869-95-EPP 220869-6-PP, 220869-07-6P 220869-10-PP 220869-10-PP 220869-18-PP 220869-18-PP 220869-18-PP 220869-18-PP 220869-18-PP 220869-19-2PP 220869-19-2PP 220869-19-2PP 220869-20-7-PP 220869-27-PP 220869-20-PP 220869-30-0PP 220869-33-0P 220869-35-PP 220869-30-PP 220869-39-6P 220869-35-PP 220869-31-0PP 220869-39-6P 220869-30-PP 220869-31-0PP 220869-310-0PP 220869-31-0PP 22

220869-41-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (Jreparation of amino acid-derived thiadiazolidinone dioxide derivs.

ss serine protease inhibitors)
RN 220868-74-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-(chloromethyl)-5-[(4-methoxyphenyl)methyl]-,
1,1-dioxide (9CI) (CA INDEX NAME)

RN 220868-75-7 HCAPLUS CN 1,2,5-Thiadiarolidin-3-one, 2-(chloromethyl)-5-((3-phenoxyphenyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2C1 N S O N CH2

RN 220868-80-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(4-methoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

CH2-OAC

RN 220868-81-5 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 2-[(acetyloxy)methyl]-5-[(3phenoxyphenyl]methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

O = 5-Me

CH2-N-C-OME

O O O

N

CH2

Pho

Absolute stereochemistry.

RN 220868-92-8 HCAPLUS
CN L-Phenylalanine,
4-chlor-N-[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl]- (9CI) (CA INDEX NAME)

MeO N S H S CO2H CI

RN 220868-93-9 HCAPLUS
CN L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl])methyl]-1,2,5-thiadiazolidin-2-yl]methyl]thio]methyl][9CI]
(GCA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CH2-OAC

RN 220868-86-0 HCAPLUS
Carbamic acid, [[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3-oxo-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 220868-87-1 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

Pho Soo H SOO2H CO2H

RN 220868-98-4 HCAPLUS
CN L-Phenylalanine,
4-chloro-N-[[[5-[(4-methoxyphenyl)methyl]-1,1-dioxido-3oxo-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220868-99-5 HCAPLUS
L-Phenylalanine, 4-chloro-N-[[[[1,1-dioxido-3-oxo-5-[(3-phenoxyphenyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]sulfonyl]methyl]- (SCI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-05-6 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5thiadiazolidin-2-yl)methyl](phenylsulfonyl)-, methyl ester (9CI) [CA
INDEX NAME)

220869-06-7 HCAPLUS
Carbanic acid, {[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl}(phenylsulfonyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

RN 220869-16-9 HCAPLUS
CN Carbamic acid,
[2-{[4-(2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiacolidin-2-yl]methyl](methylsulfonyl)amino]-2-oxoethyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

RN 220869-19-2 HCAPLUS
CN Glycine,
[[[[4-[2-methylpropy1]-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5thiadiazolidin-2-yl]methyl] [phenylsulfonyl)amino]carbonyl)-, ethyl ester
(961) (CA INDEX NAME)

220869-20-5 HCAPLUS
1,2,5-Thiadiacolidin-3-one, 2,2'-methylenebis(4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1,1',1'-tetraoxide (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-07-8 HCAPLUS
Carbamic acid, [[1,1-dioxido-3-oxo-4,5-bis(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl](methylsulfonyl)-, butyl ester (9CI) (CA INDEX

NAME)

RN 220869-14-7 HCAPLUS
CN Carbamic acid,
[2-{[[4-{2-methylpropyl}-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl](methylaulfonyl)amino]-2-oxoethyl]-,
1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-26-1 HCAPLUS
1,2,5-Thiadizolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4-(2-methylpropyl)-5-[phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 220869-27-2 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[(4,5-diphenyl2-2-oxazoly1)|thio]methyl]-4-(2methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-29-4 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-[[(5-

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Contphenyl-1,3,4-oxadiazol-2-yl)thio]methyl]-, 1,1-dioxide (9CI) NAME) (Continued)

220869-30-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[(2-benzothiazolylthio)methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-33-0 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-(phenylmethyl)-2-[[(3-phenyl-1,2,4-oxadiazol-5-yl)thio]methyl}-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-40-9 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-[[(6-amino-2-benzoxazolyl)thio]methyl]-4,5-bis[[henylmethyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

NAME)

Absolute stereochemistry.

220869-64-7 220869-65-8 RL: RCT (Reactant) / RRCT (Reactant) or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derive. ΙT

serine protesse inhibitors) 220869-64-7 HCAPLUS

1.2.5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-,

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-35-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-2-[[(5-phenyl-2-benzoxazolyl)thio]methyl}-5-(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX

220869-38-5 HCAPLUS 1,2,5-Thiadizcolidin-3-one, 2-[(2-benzoxazolylthio)methyl]-4,5-bis[(phenylmethyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

220869-39-6 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[((5-phenyl-1,3,4-oxadiazol-2-yl)thio]methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

220869-65-8 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-, 1,1-dioxide, (45)-(9CI) (CA INDEX NAME) (45)-

220869-61-4P 220869-62-5P 220869-63-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of amino acid-derived thiadiazolidinone dioxide derivs. IT

serine protease inhibitors)

220869-61-4 HCAPLUS

1.2.5-Thiadiarolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5(phenylmethyl)-, 1,1-dimethylethyl ester, 1,1-dioxide, (45)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

220869-62-5 HCAPLUS
1,2,5-Thiadiazolidine-2-acetic acid, 4-(2-methylpropyl)-3-oxo-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

220869-63-6 HCAPLUS 1,2,5-Thiadiacolidine-2-acetamide, 4-(2-methylpropyl)-3-oxo-N-(2-phenylethyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9C1) (CA IND (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued 212331-98-1 KCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-((phenylthio)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212331-99-2 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 2-(chloromethyl)-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

212332-00-8 HCAPLUS
Benzeneacetic acid, 3-[((35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylthio)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA INDEX

Absolute stereochemistry

IT 212331-79-8P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3) 212331-79-8 HCAPLUS

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 05 Aug 1998 ACCESSION NUMBER: 1998:487562 HCAPLUS DOCUMENT NUMBER: 129:216561

129:216561
Potent and specific inhibition of human leukocyte elastase, cathepsin G and proteinase 3 by sulfone derivatives employing the 1,2.5-thiadiazolidin-3-one 1,1-dioxide scaffold Groutas, William C.; Kuang, Rongze; Ruan, Sumei; Epp, Jeffrey B.; Venkataraman, Radhika; Truong, Tien M. Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA Bioorganic 4 Medicinal Chemistry (1998), 6(6), AUTHOR (S): CORPORATE SOURCE:

SOURCE: 661-671

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Science Ltd.

PUBLISHER: Journal English

DOCUMENT TYPE: LANGUAGE:

TITLE:

This paper describes the results of structure-activity relationship studies in a series of heterocyclic mechanism-based inhibitors based on the 1,2,5-thiadiazolidin-3-one 1,1-dioxide scaffold (1; R1 = iso-6benzyl: R2 = Bu, Me, benzyl; R2 = Bu, Me, benzyl; R2 = Bo; Me, benzyl; R5 = SoZPh, SOZC6H4Cl-4, etc.) and capable of interacting with the Sn and S'n subsites of a serine proteinase. Sulfone derivs. of I were found to be highly effective, time-dependent inhibitors of human leukocyte elastase (HLE), cathepsin G (Cat G) and proteinase 3 (PR 3). The judicious selection of an R1 group (accommodated at the primary specificity site S1) that is based on the known substrate specificity of a target serine proteinase, was found to yield highly selective inhibitors. The presence of a benzyl group (R2 = benzyl) at the S2 subsite was found to lead to a pronounced enhancement

inhibitory potency. Furthermore, the effective use of computer graphics and modeling has led to the design of potent, water-soluble inhibitors.

The
results of these studies demonstrate that the 1,2,5-thiadiazolidin-3-one
1,1-dioxide platform provides an effective means for appending
recognition
elements in a well-defined vector relationship, and in fashioning
highly-selective and potent inhibitors of serine proteinases.

If 212331-98-1P 212331-99-2P 212332-00-8P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(1,2,5-thiadiazolidin-3-one 1,1-dioxide inhibitors of human leukocyte
elastase, cathepsin G and proteinase 3)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 AC5 on STN (Continued)
Benzoic acid, 3-[[(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

IT 170918-99-7P 170919-01-4P 170919-03-6P
212331-77-6P 212331-78-7P 212331-80-1P
212331-81-2P 212331-82-3P 212331-83-4P
212331-86-7P 212331-89-8P 212331-95-8P
212331-97-0P
R1: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation as inhibitor of human leukocyte elastase, cathepsin G and proteinase 3)
RN 170918-99-7 MCAPUUS
CN 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2((phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

170919-01-4 HCAPLUS
1, 2, 5-Thiadiazolidin-3-one,
(phenylmethyl)-5-([25]-3-phenyl-2-propenyl)2-{(phenylmulfonyl)methyl}-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Ph S N E Ph

RN 170919-03-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

N 212331-77-6 HCAPLUS
N Benzoic acid, 4-[(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl)-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-78-7 HCAPLUS
CN Benzoic acid, 4-[([35)-3-{2-methylpropyl)-1,1-dioxido-4-oxo-5-[(phenylsulfonyl)methyl)-1,2,5-thiadiazolidin-2-yl]methyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 212331-62-3 HCAPLUS
CN Benzoic acid, 2-[{(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-83-4 HCAPLUS

Benzeneacetic acid, 4-[{(35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-86-7 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 2-[[(4-chlorophenyl)sulfonyl]methyl]-4-(2-methylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

RN 212331-80-1 HCAPLUS

Benzoic acid, 3-[([35)-3-(2-methylpropyl)-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 212331-81-2 HCAPLUS
CN Benzoic acid, 2-[[(35)-3-{2-methylpropyl}-1,1-dioxido-4-oxo-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl]methyl]-, methyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued Absolute stereochemistry.

RN 212331-87-8 HCAPLUS CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(2-phenylethyl)-2-[(phenylsulfonyl]methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 212331-90-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
2-[[[(4-chlorophenyl)methyl]sulfonyl]methyl]-4(2-ethylpropyl)-5-(phenylmethyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

212331-92-5 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-{2-methylpropyl}-5-{phenylmethyl}-2-[[(3-phenylpropyl)sulfonyl]methyl]-, 1,1-dioxide, (4S)- {9CI} (CA INDEX NAME)

RN CN

212331-94-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2-{{[3-(trifluoromethyl)phenyl]sulfonyl]methyl}-, 1,1-dioxide, (45)- (9CI) · (CA INDEX NAME)

Absolute stereochemistry.

212331-95-8 HCAPLUS

212331-95-0 MCAPLUS 1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2-[(phenylsulfonyl]methyl]-, 1,1-dioxide, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 09 Apr 1998 ACCESSION NUMBER: 1998:200895 HCAPLUS

1998:200895 HCAPLUS 128:278642 DOCUMENT NUMBER:

TITLE:

128:278642
Use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent inhibitors of serine proteinases Kuang, Rongze: Venkataraman, Radhika; Ruan, Sumei: Groutas, William C.
Department of Chemistry, Wichita State University, Wichita, KS, 67260, USA
Bioorganic & Medicinal Chemistry Letters (1998),

AUTHOR(S):

CORPORATE SOURCE:

SOURCE: 8(5),

539-544 CODEN: BMCLE8; ISSN: 0960-894X Elsevier Science Ltd. Journal

PUBLISHER:

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The attachment of a phosphate leaving group to the
1,2,5-thiadiazolidin-3one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds was found
to yield highly potent, time-dependent inhibitors of human leukocyte
elastase (HLE).

205932-85-0P 205932-87-2P 205932-88-3P
205932-89-4P 205932-89-3P 20593

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (use of the 1,2,5-thiadiazolidin-3-one 1,1 dioxide and isothiazolidin-3-one 1,1 dioxide scaffolds in the design of potent in the control of the control o

inhibitors of serine proteinases) 205932-85-0 HCAPLUS

205932-85-0 HCAPLUS
Phosphoric acid, dimethyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl ester (9CI) (CA INDEX

205932-87-2 HCAPLUS
Phosphoric acid, dibutyl [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl}methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

212331-97-0 HCAPLUS
Benzeneacetic acid, 4-[[(3S)-1,1-dioxido-4-oxo-3-(phenylmethyl)-5[(phenylsulfonyl)methyl]-1,2,5-thiadiazolidin-2-yl)methyl]- (9CI) (CA
INDEX NAME)

REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

205932-88-3 HCAPLUS
Phosphoric acid, [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)1,2,5-thiadiazolidin-2-yl]methyl bis(phenylmethyl), ester (9CI) (CA INDEX NAME)

205932-89-4 HCAPLUS
Phosphoric acid, [4-(2-methylpropyl)-1,1-dioxido-3-oxo-5-(phenylmethyl)-1,2,5-thiadiazolidin-2-yl]methyl diphenyl ester (9CI) (CA INDEX NAME)

THERE ARE 20 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

CORPORATE SOURCE:

L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 30 Aug 1997
ACCESSION NUMBER: 1997:555602 HCAPLUS
DOCUMENT NUMBER: 127:257045

TITLE: Competitive particle concentration fluorescence
immunoassays for measuring antidiabetic drug levels

mouse plasma
Bright, Stuart W.; Tinsley, Frank C.; Dominianni,
Samueř J.; Schmiegel, Klaus K.; Fitch, Lora L.; Gold,
Gerald
Lilly Research Laboratories, Eli Lilly and Company,
Indianapolis, IN, 46285, USA
Journal of Immunological Methods (1997), 207(1), AUTHOR (5)

CODEN: JIMMBG; ISSN: 0022-1759

PUBLISHER: DOCUMENT TYPE: LANGUAGE:

CRY TYPE: Journal NAGE: English Two competitive particle concentration fluorescence immunoassays were developed

loped to measure blood levels of analogs of antidiabetic drugs being tested in diabetic mice. Ligands that contained the active pharmacophores were conjugated to PPD for immunization and to β-phycoerythrin for use as a tracer in the immunoassays. Approx. 909 of 262 compds. assayed were detectable at less than 120 nM in plasma which was well below the

iated therapeutic level of 1 µM for lowering blood glucose. These data were used to define the bioavailability of test compds. and assist in decisions

nions of constructing active analogs. Of addnl. interest, we noted crossreactivity of one monoclonal antibody for 3 different compound

ses
that are all known to bind with varying affinities to peroxisome
proliferator-activated receptors.
196079-43-3
RL: ANT (Analyte): ANST (Analytical study)
(competitive particle concentration fluorescence immunoassays for

measuring
antidiabetic drug levels in mouse plasma)
RN 156079-43-3 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 5-[4-[2-(2-phenyl-4-oxažolyl)ethoxy]phenyl]-,
1,1-dioxide (SCI) (CA INDEX NAME)

- Bilanzo

FORMAT

THERE ARE 13 CITED REFERENCES AVAILABLE FOR 13

REFERENCE COUNT: THIS

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN
ED Entered STN: 09 Apr 1997
ACCESSION NUMBER: 1997:226843 HCAPLUS
DOCUMENT NUMBER: 126:287581
TITLE: Structure-Based Design of a Gene

Structure-Based Design of a General Class of Mechanism-Based Inhibitors of the Serine Proteinases

AUTHOR(S):

Mechanism-Based Inhibitors of the Serine Proteinases
Employing a Novel Amino Acid-Derived Heterocyclic
Scaffold
AUTHOR(S): Groutas, William C.; Kuang, Rongze; Venkataraman,
Radhika; Epp, Jeffrey B.; Ruan, Sumei; Prakash, Om
CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260, USA
Blochemistry (1997), 36(16), 4739-4750
COODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
Journal
LANGUAGE: Journal
LANGUAGE: English
AB We describe in this paper the structure-based design of a general class
of CORPORATE SOURCE:

PUBLISHER: DOCUMENT TYPE:

heterocyclic mechanism-based inhibitors of the serine proteinases that embody in their structure a novel peptidomimetic scaffold (1,2,5-thiadiazolidin-3-one 1,1-dioxide). Sulfone derivs. of this class were time-dependent, potent, and highly efficient irreversible inhibitors of human leukocyte elestase, cathepsin G, and proteinase 3. The partition

partition
ratios for a select number of inhibitors were found to range between 0
and 1.
We furthermore demonstrate that these inhibitors exhibit remarkable

We furthermore demonstrate that these inhibitors exhibit remarkable enzyme
selectivity that is dictated by the nature of the Pl residue and is consistent with the known substrate specificity reported for these enzymes. Thus, inhibitors with small hydrophobic side chains were effective inhibitors of elastase, those with aromatic side chains of cathepsin G, and those with a basic side chain of bovine trypsin. Take together, the findings cited herein reveal the emergence of a general class of stable mechanism-based inhibitors of the serine proteinases which

which

can be readily synthesized using amino acid precursors. Biochem. and
high-field NMR studies show that the interaction of this class of
inhibitors with a serine proteinase results in the formation of a stable
acyl complex(es) and the release of benzenesulfinate, formaldehyde, and a
low mol. weight heterocycle. The data are consistent with initial
formation
of a Michaelis-Menten complex, acylation of Ser195, and tandem loss of
the

leaving group. The initial HLE-inhibitor complex reacts with water generating formaldehyde and a stable HLE-inhibitor complex. Whether the initial HLE-inhibitor complex also reacts with His57 to form å third complex is not known at this point. The desirable salient parameters associated with this class of inhibitors, including the expeditious generation of structurally diverse libraries of inhibitors based on I, suggest that this class of mechanism-based inhibitors is of general applicability and can be used in the development of inhibitors of human and viral serine proteinases of clin. relevance. 170918-99-79 170919-30-69 189124-00-39
189124-02-59 189124-04-79 189124-06-99
PL: NBC (Bollogical activity or effector, except adverse); BSU

BAC (Biological activity or effector, except adverse); BSU

R1: BAC (Blological activity or effector, except accesses); bou (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and structure activity relations of mechanism-based inhibitors

L4 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) of human leukocyte serine proteinases employing a novel amino acid-derived heterocyclic scaffold)
170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-03-6 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylmulfonyl)methyl]-, 1,1-dioxide, (45)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

189124-00-3 HCAPLUS 1,2,5-Thiadiazolidin-3-one, 4-ethyl-5-(phenylmethyl)-2-((phenylsulfonyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

189124-02-5 HCAPLUS

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on 5TN CN 1,2,5-Thiadiazolidin-3-one, 5-(phenylmethyl)-2-([phenylmulfonyl)methyl]-4-propyl-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME) (Continued)

189124-04-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(1-methylethyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189124-06-9 HCAPLUS
1,2,5-Thiadiarolidin-3-one, 4-butyl-5-(phenylmethyl)-2((phenylmulfonyl)methyl)-, 1,1-dioxide, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS ON STN ED Entered STN: 01 Dec 1995 ACCESSION NUMBER: 1995.954574 HCAPLUS DOCUMENT NUMBER: 123:340140 TITLE: Novel serine protease inhibitors: derivatives of isothiazolidin-3-one 1,1-dioxide and isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide Groutas, William C. Wichita State University, USA PCT Int. Appl., 93 pp. CODEN: PIXXD2
Patent PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

												ICAT					ATE	
												995-					0050	103
we																		
	W	:										CN,						
												LT,						
			NL,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SI,	SK,	TJ,	TT,	UΑ,	UΖ,	VN
	RI	W :	AT.	BE.	CH.	DE.	DK.	ES.	FR.	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE
U:	5 5 5	50	139			A		1996	0827		US I	994-	1773	52		1	9940	103
C.	21	79	913			A1		1995	0713		CA 1	995-	2179	913		1	9950	103
Δ1	1 95	15	998			A		1995	0801		AU 1	995-	1599	В		1	9950	103
14	1 68	63	16			B2		1998	0205									
F	73	93	38			A1		1996	1030		EP 1	995-	9080	03		1	9950	103
								2002										
											CB	IE,	TT	T.T.	Tati.	MC.	NI.	PT.
		•	м,	ьь,	CII,	DE,	DK,	ь.,	ı,	UD,	٠,	+-,	,	,	,	,	,	,
SE						т		1007	1007		** 1	995-	E10 <i>E</i>	70		1	9950	103
																	9950	
						T		2002				995-						
N:	2 32	97	66			А		2001	0223			998-						
PRIORI	A Y	PP:	LN.	INFO	.:						US 1	994-	1773	52		A 1	9940	103
											WO 1	995-	US23	6		w 1	9950	103

MARPAT 123:340140 OTHER SOURCE(S):

Various isothiazolidin-3-one 1,1-dioxide and 3-oxo-1,2,5-thiadiazolidine 1,1-dioxide derivs., e.g. I [X=CR2, (un)substituted NH; R1=H, alkyl, (un)substituted NH; R1=H, alkyl, (un)substituted henzyl, indolylalkyl, etc.; Y=non-steroidal antiinflammatory residue, H, protected amino acid, acyloxy, etc.], and their use to reduce or inhibit the activity of serine proteases, are claimed. The compds. are useful as anti-inflammatory and anti-metastatic agents. For example, 4-benzylisothiazolidin-3-one 1,1-dioxide underwent

L4 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) N-alkylation with CLCH25Ph and EtNn in MeCN, followed by S-oxidn. with m-ClC6H4C(0)00H in CH2Cl2 (908), to give title compd. II. In an in vit assay, II had an apparent 2nd-order inactivation rate const. (kobs/[I])

M-1

s333, In and an apparent 2nd-order instruction that constant can be said or tested against cathepsin G. A variety of compds. were prepd. and/or tested against cathepsin G, human leukocyte elastase, and/or proteinase-3.

1 170919-16-1P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; preparation of isothiazolidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors)

RN 170919-16-1 RCAPLUS

RN 170919-16-1 RCAPLUS

CN 1.2,5-Thiadiazolidin-3-one, 4-(phenylmethyl)-5-(3-phenyl-2-propenyl)-2-(phenylthio)methyl]-, 1,1-dioxide, [S-(E)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

IT 170919-15-0P
R1: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-15-0 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4,5-bis(phenylaethyl)-2-[(phenylthio)methyl]-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 153044-45-2P 170918-99-7P 170919-01-4P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued) study, unclassified; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Blological study); PREP (Preparation); USES (Uses) (prepn. of isothiazollidinone and oxothiadiazolidine dioxide derivs. as serine protease inhibitors) 153044-45-2 HCAPLUS 1,2,5-Thiadiazollidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-, 1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

170918-99-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4,5-bis(phenylmethyl)-2[(phenylsulfonyl)methyl]-, 1,1-dioxide, (45)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 170919-01-4 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one,
4-(phenylmethyl)-5-[(2E)-3-phenyl-2-propenyl]2-[(phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

170919-22-9 HCAPLUS 1/2,5-Thiadiazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 170919-03-6 170919-21-8 170919-22-9
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Uses)
(preparation of isothiazolidinone and oxothiadiazolidine dioxide
derivs. as
serine protease inhibitors)
RN 170919-03-6 HCAPLUS
CN 1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2((phenylsulfonyl)methyl]-, 1,1-dioxide, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

170919-21-8 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-(2-methylpropyl)-5-(phenylmethyl)-2[(phenylsulfonyl)methyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 19 Mar 1994
ACCESSION NUMBER: 1994:124451 HCAPLUS
DOCUMENT NUMBER: 120:124451
TITLE: 5 Substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides:
a new class of potential mechanism-based inhibitors

of

AUTHOR(S):

human leukocyte elastase and cathepsin G Groutas, William C.; Kuang, Rongze; Venkataraman, Radhika Dep. Chem., Wichita State Univ., Wichita, KS, 67260, USA Biochemical and Biophysical Research Communications (1994), 198(1), 341-9 CODEN: BBRCA9; ISSN: 0006-291X Journal English CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: GI

A series of substituted 3-oxo-1,2,5-thiadiazolidine 1,1-dioxides (I, R = benzyl; Rl = H, Me, benzyl, CH2CO2-tert-Bu or CH2CO2-benzyl) was prepd, and their in vitro inhibitory activity toward human leukocyte elastase

and

cathepsin G was investigated. These compds. inactivated the 2 enzymes efficiently and in a time-dependent fashion.

IT 153044-45-2P
RL: SPN [Synthetic preparation]; PREP (Preparation)
(preparation of and human leukocyte elastase and cathepsin G inhibition by)
RN 153044-45-2 HCAPLUS
CN 1,2,5-Thiediazolidin-3-one, 2-(fluoromethyl)-4,5-bis(phenylmethyl)-,
1,1-dioxide, (S)- (9CI) (CA INDEX NAME)

L4 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 26 Jan 1991
ACCESSION NUMBER: 1991:23940 HCAPLUS
DOCUMENT NUMBER: 114:23940
TITLE: 114:23940
TITLE: 116:23940 HCAPLUS
TITLE: 116:23940 HCAPLUS

AUTHOR(S): CORPORATE SOURCE:

Lee, Chai Ho; Kohn, Harold Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA

USA Journal of Organic Chemistry (1990), 55(25), 6098-104 CODEN: JOCEAH; ISSN: 0022-3263 Journal English CASREACT 114:23940 SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(5): GI

The utility of $\alpha\text{-sulfamidoalkylation}$ processes for the generation of sulfamides has been examined. Both intra- and intermol. $\alpha\text{-}$ sulfamidoalkylation transformations were observed to proceed in moderate

good yields. The generality of these processes has been demonstrated using N.N'-di(aryl-substituted)sulfamides, and the utility of these reactions was examined for the preparation of cyclic sulfamides of novel structure. Thus, reaction of PhoRNINSO2NIE with EcoZCCH(OBL)2 in the presence of CF3COZH gave 74% dithiatetrazocinedicarboxylate tetraoxide I, whereas reaction of 3-MeOC644CH2NHSO2NHZ with EtOZCCH(OBL)2 in CF3COZH followed by methylation gave benzothiadiazepinecarboxylate dioxide II. The crystal structures of I and II were determined 130670-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of) 130670-00-7 HCAPLUS
1,2,5-Thiadiazolidin-3-one, 4-hydroxy-5-(2-phenylethyl)-, 1,1-dioxide, monosodium salt (9CI) (CA INDEX NAME)

ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

• Na

130669-99-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) [preparation and hydride reduction of) 130669-99-7 HCAPLUS [1,2,5-Thiadiazolidine-3,4-dione, 2-(2-phenylethyl)-, 1,1-dioxide, sodium salt (9CI) (CA INDEX NAME)

• Na

=> log y		
=> log y COST IN U.S. DOLLARS	SINCE FILE	TOTAL
•	ENTRY	SESSION
FULL ESTIMATED COST	173.69	340.84
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-24.75	-24.75

STN INTERNATIONAL LOGOFF AT 12:20:59 ON 21 DEC 2006